A Rigorous Landauer-Büttiker Formula and its Application to Models of a Quantum Dot LED

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Abstract

The subject of this thesis is the modeling of a quantum dot LED and the calculation of the electric current and the light production in the Landauer-Büttiker framework.

The electron-photon interaction is fitted into the Landauer-Büttiker framework by assuming that every electron interacts with a separate photon field. It allows us to consider an electron together with its photon field as a 'single non-interacting particle' in the sense of the Landauer-Büttiker formalism.

We develop a model of a QD-LED with an electron-photon interaction that is based on the Jaynes-Cummings model, which describes the interaction of a quantum dot with a single mode of the electromagnetic field. To be able to analyze the energy distribution of the emitted photons, we propose a second model of a QD-LED that is based on a one-dimensional Pauli-Fierz model. It models photons of arbitrary positive energy instead of just a single mode, but we restrict it to the subspace of at most one photon.

We prove an abstract Landauer-Büttiker formula that applies to all relatively trace class scattering systems. It is similar to the result by Aschbacher et al. (2007), but differs in the regularization of the flux. Furthermore, our proof uses an explicit spectral representation, which makes it more transparent. We apply this abstract result to the Jaynes-Cummings QD-LED.

Since the knowledge of the scattering matrix is essential for explicit calculations with the Landauer-Büttiker formula, we generalize a result by Behrndt et al. (2010) on a representation of the scattering matrix in terms of the Weyl function of a boundary triplet from the finite rank case to relatively trace class perturbations, which covers the case of the Jaynes-Cummings QD-LED.

The resolvent difference of the Pauli-Fierz QD-LED is not trace class, whence we prove a generalized Landauer-Büttiker formula for a certain class of multiplication operators that are trace class in the fiber. This abstract result gives us a Landauer-Büttiker formula also for the Pauli-Fierz QD-LED.

Zusammenfassung

Die vorliegende Arbeit behandelt die Modellierung einer Quantenpunkt-LED und die Berechnung des elektrischen Stromes und der Lichtproduktion im Landauer-Büttiker-Formalismus.

Die Elektron-Photon-Wechselwirkung kann im Landauer-Büttiker-Formalismus behandelt werden, indem wir annehmen, dass jedes Elektron mit einem separaten Photonenfeld interagiert. Dies erlaubt es uns, ein Elektron zusammen mit seinem Photonenfeld als "einzelnes, nicht wechselwirkendes Teilchen" im Sinne des Landauer-Büttiker-Formalismusses zu betrachten.

Wir entwickeln ein Modell einer QP-LED, dessen Elektron-Photon-Wechselwirkung auf dem Jaynes-Cummings-Modell basiert. Dieses beschreibt die Wechselwirkung eines Quantenpunkts mit einer einzelnen Mode des elektromagnetischen Feldes. Um auch die Energieverteilung der emittierten Photonen analysieren zu können, schlagen wir ein zweites QP-LED-Modell vor, das auf einem eindimensionalen Pauli-Fierz-Modell basiert. Anstelle einer einzelnen Mode modelliert es Photonen beliebiger Energie, allerdings beschränken wir uns auf den Unterraum mit maximal einem Photon.

Wir beweisen eine abstrakte Landauer-Büttiker-Formel, die für alle relativ nuklearen Streusysteme gilt. Sie ist ähnlich zu dem Ergebnis von Aschbacher et al. (2007), unterscheidet sich aber in der Regularisierung des Stroms. Außerdem nutzt unser Beweis eine explizite Spektraldarstellung, wodurch er klarer wird. Wir wenden das abstrakte Ergebnis auf die Jaynes-Cummings-QP-LED an.

Da die Kenntnis der Streumatrix für explizite Berechnungen mit der Landauer-Büttiker-Formel notwendig ist, verallgemeinern wir die Darstellung der Streumatrix durch die Weyl-Funktion eines Randwert-Triplets von Behrndt et al. (2010) vom Fall für Störungen endlichen Ranges auf den Fall relativ nuklearer Störungen. Dies deckt insbesondere den Fall der Jaynes-Cummings-QP-LED ab.

Die Resolventendifferenz der Pauli-Fierz-QP-LED ist nicht nuklear, weshalb wir eine verallgemeinerte Landauer-Büttiker-Formel für eine gewisse Klasse von Multiplikationsoperatoren beweisen, die in der Faser nuklear sind. Dieses abstrakte Resultat liefert uns auch für die Pauli-Fierz-QP-LED eine Landauer-Büttiker-Formel.

Contents

1 Introduction

Semiconductor quantum devices such as quantum wells, nanowires, and quantum dots have become more and more popular areas of research over the last decade. With the improvement of production technologies, the properties of these devices can be fine-tuned, thus opening a wider range of applications.

Our special interest lies in *quantum dots*. Quantum dots are nano objects — e.g. pyramids made of semiconductor material, cf. Figure 1.1 — that confine electrons in all three spatial dimensions, which results in a discrete energy spectrum. This is why they are sometimes called *artificial atoms*.

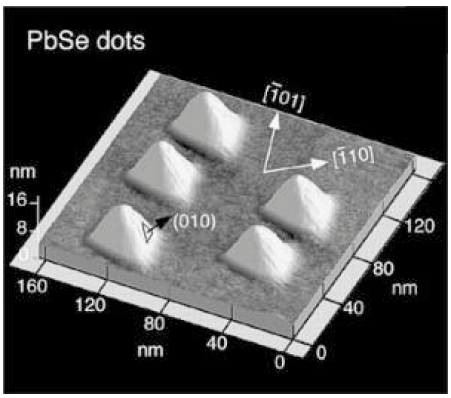

Figure 1.1: PbSe quantum dots, taken from Springholz et al. [77]

They have a wide range of applications in electronics and optics, e.g. single electron transistors and quantum dot lasers. We focus on the optoelectronic properties with non-coherent light, like in quantum dot light emitting diodes, but also quantum dot solar cells. Since the exact properties are not essential for the mathematics, we use the term quantum dot light emitting devices to refer to the quantum system under consideration, QD-LEDs for short. The physical properties of such devices have been studied in various publications. Ryzhii [73] investigated quantum dot phototransistors, Ryzhii and Khmyrova [74] used quantum dots as photodetectors and LEDs. By creating quantum dots of a specific size, the emission spectrum of the quantum dot LED can be tuned very precisely. Thus, the whole range of colors in the visible spectrum can be realized. This opens up the possibility to use quantum dot LEDs as red, green, and blue pixel elements in a color display [21, 22, 78]. The pixels are actively emitting light, as opposed to conventional LCD displays, where the colors are created by filtering the white background light. This allows high contrasts. Additionally, the emission spectrum of quantum dots is very narrow, which enables quantum dot LED displays to render colors much more accurately than conventional LCD displays. The tunability of the quantum dots is also of great use in quantum dot solar cells [7, 75, 33]. It makes it possible to

build solar cells that can absorb a wide range of photon frequencies, thus increasing the efficiency. For quantum dot LEDs it is obviously of interest to calculate the light production of the LED and the current necessary to produce this light. For solar cells, the electric current is most important, but the photon absorption is also of interest.

The main topic of this thesis is the formulation of abstract models for a QD-LED and the calculation of the electric current and the photon production rate. The central concept we use is the Landauer-Büttiker formalism.

1.1 Landauer-Büttiker formula

The Landauer-Büttiker formula is originally a tool to calculate the steady state current through a quantum device that is contacted by two leads with a potential bias, i.e. an applied voltage. The concept immediately generalizes to an arbitrary number of leads and an arbitrary number of conducting channels in each lead. The invention of this formalism is due to Landauer [61], and the principal work on this is [18]. The main modeling idea is to neglect the Coulomb interaction of the electrons, i.e. to treat the electrons as non-interacting particles. This way it suffices to consider the transport of a single electron through the quantum system since every electron of equal energy will behave the same, irrespective of the presence of other electrons. Thus, the current from one lead to another is determined by the number of electrons in the one lead times the probability of the electron to travel through the quantum system into the other lead. This probability is given by the scattering cross-section $\sigma(\lambda)$, which can be obtained from the scattering matrix. Thus, the problem of calculating the current is put into the framework of scattering theory and reduced to the calculation of the scattering matrix. A drawback of this approach is that certain interesting phenomena are not captured by this model. For example, the increase of the differential resistance at small voltage bias caused by the Coulomb interaction, called Coulomb blockade, can not be described by non-interacting electrons.

In order to speak of a scattering matrix, one has to identify the scattering system $\{H_0, H\}$. Recall that a scattering system is a pair $\{H_0, H\}$ of Hamiltonians, where the *interacting* Hamiltonian H describes the real physical system and the *free* Hamiltonian H_0 describes the asymptotic evolution of the system. The fundamentals of mathematical scattering theory can be found in Appendix A.2. In the case of a contacted quantum device, the interacting Hamiltonian H is of course given by the system under consideration. However, the free Hamiltonian H_0 can be chosen with certain freedom. There are two fundamentally different approaches. One concept is to start with zero potential bias and then increase the bias adiabatically. This is the so-called *partition-free approach* introduced by Cini [20]. It has been further analyzed by Cornean et al. [25, 27, 28]. The main difficulty is that the perturbation $H - H_0$ is non-local.

The second idea is to start with decoupled subsystems that are individually in equilibrium. This idea goes back to Caroli et al. [19] and Ruelle [72]. Initially, the system consists of the leads and the quantum system, which are isolated from each other. This is described by the Hamiltonian H_0, which decomposes into a direct sum of the Hamiltonians of the subsystems. Every subsystem is in equilibrium, but not necessarily with the same chemical potential. The leads are then coupled in such a way that one obtains

the interacting Hamiltonian H that describes the real physical system in which the current flows. It has been proven by Cornean et al. [26] that the manner of the coupling, suddenly or adiabatically, has no impact on the resulting steady state current. Since the perturbation is local in this approach, the scattering theory is considerably easier. This concept of initially decoupled subsystems is the one that we use throughout this thesis.

Let us take the simple example of one-dimensional electrons with two leads l and r coupled to a double barrier quantum system S, cf. Figure 1.2. It is described by the Hamiltonians $H_j = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + v_j(x)$, $j \in \{l, S, r\}$. The applied bias is modeled by a difference in the chemical potentials μ_l and μ_r of the leads. An applied voltage does of course affect the potential. We assume that the potentials v_l and v_r are constant in the leads and $v_S(x)$ is the potential under the applied voltage. The equilibrium states of the leads are $\rho_j = f_{FD}(H_j - \mu_j)$, $j \in \{l, r\}$, where $f_{FD}(\lambda) = (1 + e^{\beta\lambda})^{-1}$ is the Fermi-Dirac distribution function with inverse temperature $\beta \in (0, \infty]$, cf. Equation A.1.11 in the appendix. In other words, the probability for an electron in lead j to have energy λ is $f_{FD}(\lambda - \mu_j)$.

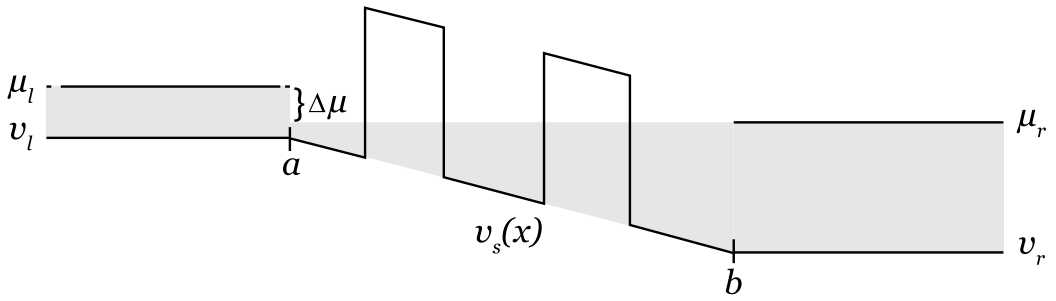

Figure 1.2: One-dimensional double barrier contacted with leads

For a fixed energy λ, the probability for an electron to pass from lead l through the quantum system to lead r is $\sigma_{lr}(\lambda) = |T_{lr}(\lambda)|^2$, where $T_{lr}(\lambda)$ is the off-diagonal element of the symmetric 2×2-matrix $T(\lambda)$, the transition matrix (cf. Appendix A.2). Hence, by the heuristic argument above, the current density of the current from lead l to lead r is proportional to $f_{FD}(\lambda - \mu_l)\sigma_{lr}(\lambda)$. Vice versa, the current density from r to l is proportional to $f_{FD}(\lambda - \mu_r)\sigma_{lr}(\lambda)$. Then the net current flowing into the lead l is

$$\mathfrak{J} = -2\pi \int_{\mathbb{R}} \mathrm{d}\lambda\, \sigma_{lr}(\lambda)(f_{FD}(\lambda - \mu_r) - f_{FD}(\lambda - \mu_l)). \tag{1.1}$$

In the case of zero temperature, we have $\beta = \infty$ and hence

$$f_{FD}(\lambda - \mu_l) - f_{FD}(\lambda - \mu_r) = \begin{cases} 0 & \mu \notin (\mu_r, \mu_l) \\ 1 & \mu \in (\mu_r, \mu_l) \end{cases},$$

whence only the energy range $[\mu_r, \mu_l]$ between the chemical potentials is relevant for the current. Formula (1.1) can also be modified to yield the heat flux, the energy flux, and the entropy production rate of such a contacted quantum system in a non-equilibrium

steady state [2]. Let us stress that the Landauer-Büttiker formula only covers the steady state case. Transient currents, i.e. time-dependent fluctuations in the current, can not be determined by this. So far, in the literature the Landauer-Büttiker formula has only been used to calculate electron currents. Naturally, in the context of quantum dot LEDs and, in particular, of quantum dot solar cells, the electron current is also of interest — especially the impact of the electron-photon interaction on the electric current. However, for a quantum dot LED, the most important quantity is the photon production that is caused by a steady current through the quantum dot. In this thesis we present a novel approach that allows us to calculate the electron current as well as the photon production in a Landauer-Büttiker framework.

1.2 The principal modeling ideas for a quantum dot LED

Although the questions of current and light emission in contacted quantum dots is of high interest, up to now there is little work on this topic in the literature. Pedersen and Büttiker [67] and Kuo [58] both calculate the effect of photons on the electric current, but they do not analyze the light emission. To our knowledge the present thesis is the first mathematical publication devoted to the calculation of the photon production in QD-LEDs. Our main new idea is to cast the problem of modeling a QD-LED in the Landauer-Büttiker formalism. Since this formalism is based on the assumption of non-interacting particles, but the inclusion of the electron-photon interaction is obviously crucial for the behavior of the system, we have to find some modeling approach that unites the electron-photon interaction with the concept of non-interacting particles. Of course, this contradiction can only be resolved if we use some approximation. Our key idea is that of an individual photon field for each electron.

The standard space for the modeling of a many-electron system is the Fermi-Fock space $\mathfrak{F}_-(\mathfrak{h}^{el})$, where $\mathfrak{h}^{el}$ is the single-electron space. Photons can be modeled on the Bose-Fock space $\mathfrak{h}^{ph} = \mathfrak{F}_+(\mathfrak{h}_1^{ph})$ with single-photon space $\mathfrak{h}_1^{ph}$. The total Hilbert space for an electron-photon system with an arbitrary, possibly infinite number of particles is then given by the tensor product $\mathfrak{F}_-(\mathfrak{h}^{el}) \otimes \mathfrak{F}_+(\mathfrak{h}_1^{ph})$. For an overview of Fock spaces and second quantization, we refer to the Appendix A.1. A summary of the notation used in this thesis is presented at the end of this introduction in Section 1.3.1. Assume that we have free photons and non-interacting electrons, just as in the purely electric case. If we introduce an electron-photon interaction, the following can happen. An electron emits a photon that is in turn absorbed by a different electron. The net effect of this is an electron-electron interaction that is mediated by the photons, whence we no longer have non-interacting electrons. If we want to neglect this effective electron-electron interaction, we can assume that every electron interacts with a separate photon field. This way, photons emitted by an electron can not be absorbed by a different electron, whence the photons do not mediate an interaction. Physically, we assume that the photons immediately leave the quantum dot and thus can not interact with the electrons after the emission.

How can we realize this in a mathematical model? A single electron with its separate photon field can be modeled with the Hilbert space $\mathfrak{h}^{el} \otimes \mathfrak{h}^{ph}$. Our principal modeling idea is to take this system of a single electron with a photon field as a 'single particle' in

the sense of the Landauer-Büttiker formalism. A many-particle system of these fermionic 'particles' can be modeled using the space $\mathfrak{F}_-(\mathfrak{h}^{el} \otimes \mathfrak{h}^{ph})$. This approach greatly simplifies the treatment of a QD-LED and, to our knowledge, has not yet been presented in the literature. We can now model the QD-LED by choosing a suitable Hamiltonian H acting on $\mathfrak{h}^{el} \otimes \mathfrak{h}^{ph}$ that incorporates the electron-photon interaction. A system of non-interacting electrons with separate photon fields is then described by the second quantization $\mathrm{d}\Gamma(H)$. And just as in the case of non-interacting electrons, the problem can be reduced to the single-particle space $\mathfrak{h}^{el} \otimes \mathfrak{h}^{ph}$ using a density operator $\rho \in \mathfrak{B}(\mathfrak{h}^{el} \otimes \mathfrak{h}^{ph})$, cf. Section 3.1.1. The expectation value of an observable $\mathrm{d}\Gamma(Q)$, where $Q \in \mathfrak{L}_1(\mathfrak{h}^{el} \otimes \mathfrak{h}^{ph})$ is a trace class operator, is then given by the trace $\mathrm{Tr}_{\mathfrak{h}^{el} \otimes \mathfrak{h}^{ph}}(\rho\, Q)$. Let us stress again that although the Hilbert space $\mathfrak{h}^{el} \otimes \mathfrak{h}^{ph}$ is that of a single electron, the density operator ρ describes infinitely many electrons, each together with its photon field.

A very useful picture of this modeling approach is to imagine that every electron carries a backpack filled with a certain number of photons. The emission of a photon corresponds to the electron putting a part of its own energy into the backpack. When absorbing a photon, the electron takes an energy package out of the backpack and adds it to its own energy. This backpack basically introduces an additional label to the electrons. Similarly to the spin, an electron is labeled by the number of photons it is carrying.

An important aspect of this modeling approach is that the Pauli principle holds for the electron together with its photon field. If the system is in a state $(\lambda^{el}, \lambda^{ph})$ with electron energy λ^{el} and photon energy λ^{ph}, the Pauli principle should imply that the state $(\lambda^{el}, \widetilde{\lambda}^{ph})$ with $\widetilde{\lambda}^{ph} \neq \lambda^{ph}$ can not be occupied since the electron is a fermion. But in our model the electron together with the photons is considered to be a fermion, whence $(\lambda^{el}, \lambda^{ph})$ and $(\lambda^{el}, \widetilde{\lambda}^{ph})$ are two different states that can be occupied at the same time. In our backpack picture, the electrons can be distinguished by the number of photons they are carrying. This has consequences in the calculation of the photon production rate, as we will see in Section 3.2.2. We will see that the fact that we have an inexhaustible supply of electrons that emit photons causes a positive photon production rate even without a potential bias (cf. Proposition 3.2.22).

When analyzing the effect of the electron-photon interaction on the electric current in a quantum device contacted by leads, it is common to consider the quantum device together with the photon field as a black box that is connected to purely electric leads [58]. In other words, the photons do not exist outside of the quantum device. This is not a suitable setting for us since we also want to measure the photon production rate, i.e. the photon flux. As we will see in Chapter 3, the fluxes are measured in the leads and not in the quantum device. But if the photons do not exist outside of the quantum device, we are not able to measure a photon flux. Thus, we really do have to take $\mathfrak{h}^{el} \otimes \mathfrak{h}^{ph}$, where the photon Hilbert space is attached to every electric subsystem, not just to the quantum device.

1.3 Overview of the thesis

The question of how to model the interaction between electrons and photons is addressed in Chapter 2. Since the physical model of non-relativistic quantum electrodynamics is

mathematically far too complex to be tractable, we need to use different approaches. A first useful simplification are models of the Pauli-Fierz type. Another very simple but physically interesting model is the Jaynes-Cummings model that describes the interaction of a two-level electron system in a cavity with a single mode of the electromagnetic field. It is mathematically not too difficult since it is explicitly diagonalizable and the electron-photon interaction is a perturbation that is relatively trace class.

In Chapter 3, as the first main result of this thesis, we derive an abstract Landauer-Büttiker formula for relatively trace class perturbations. We then construct a model for a QD-LED based on the Jaynes-Cummings model. The mathematical simplicity of this model makes it possible to apply the abstract Landauer-Büttiker formula. This immediately results in a theorem that gives us formulae for the electric current and the photon production rate that only depend on the initial state and the scattering matrix.

To actually calculate the electric current and the photon production rate, it is necessary to compute the scattering matrix $S(\lambda)$ or, equivalently, the transition matrix $T(\lambda)$. We derive a formula for the scattering matrix in terms of the Weyl function of a suitable boundary triplet in Chapter 4, which is the second main result of this thesis. We construct a boundary triplet for the QD-LED based on the Jaynes-Cummings model such that the Weyl function is essentially the resolvent of the unperturbed system, which can be calculated explicitly. This is a useful formula for the numerical calculation of the transition matrix. Furthermore, we give an explicit analytic calculation of the transition matrix for a special case of the Jaynes-Cummings QD-LED.

We already mentioned that the width of the spectrum of the light emitted by the quantum system is of great interest in applications. To analyze this one needs models that allow a continuous range of photon energies, as opposed to the Jaynes-Cummings model. Models of the Pauli-Fierz type are suitable for this since they are closer to the standard model of non-relativistic quantum electrodynamics. In Chapter 5 we propose a model of a QD-LED based on a Pauli-Fierz model, but we restrict it to the subspace of at most one photon to keep it mathematically tractable. In this situation the electron-photon interaction is again a perturbation that is relatively trace class. However, this is no longer true for the coupling of the leads to the quantum dot, which becomes a multiplication operator that is relatively trace class in the fiber. The third main result of this thesis is the derivation of a Landauer-Büttiker formula for a certain class of multiplication operators. This abstract result can be applied to the Pauli-Fierz QD-LED, which leads to a theorem that gives us formulae for the electric current and the photon production rate.

We close this thesis with Chapter 6, where we summarize the results and difficulties of this thesis and draw conclusions relating to further work on this subject.

1.3.1 Notation

Numbers The natural numbers are denoted by $\mathbb{N} = \{1, 2, \ldots\}$ and $\mathbb{N}_0 = \{0, 1, 2, \ldots\}$. We write $\mathbb{Z}$ for the integers, $\mathbb{R}$ for the reals, and $\mathbb{C}$ for the complex numbers. The half-lines are denoted by $\mathbb{R}_\pm = \{x \in \mathbb{R} \,|\, \pm x > 0\}$ and the upper complex half-plane by $\mathbb{C}_+ = \{x + iy \in \mathbb{C} \,|\, y > 0\}$. Furthermore, $\mathbb{R}^0_\pm = \mathbb{R}_\pm \cup \{0\}$. Note that $i \in \mathbb{C}$ is always the imaginary unit. The real and imaginary part of $z \in \mathbb{C}$ are $\Re\mathrm{e}(z)$ and $\Im\mathrm{m}(z)$. The complex conjugate of z is $\overline{z}$. Finally, ϵ and δ are used for small positive real numbers.

Hilbert spaces In this thesis $\mathfrak{h}$, $\mathfrak{H}$, $\mathfrak{K}$, and $\mathcal{H}$, possibly with sub- or superscripts, are always Hilbert spaces. $\langle\cdot,\cdot\rangle$ denotes the inner product and is anti-linear in the first component and linear in the second component, corresponding to the convention in physics. All Hilbert spaces in this thesis are assumed to be separable. For a subset $\mathcal{K} \in \mathfrak{H}$, its linear span is denoted by $\mathrm{span}(\mathcal{K})$ and the closure of a linear set $\mathcal{L}$ with respect to a norm $\|\cdot\|$ is $\mathrm{clo}_{\|\cdot\|}(\mathcal{L})$. We write $\mathrm{clo}(\mathcal{L}) = \mathrm{clo}_{\|\cdot\|_{\mathfrak{H}}}(\mathcal{L})$ if $\mathcal{L}$ is defined as a subset of $\mathfrak{H}$. If $\mathfrak{K}$ is a subspace of $\mathfrak{H}$, we denote the projection of $\mathfrak{H}$ onto $\mathfrak{K}$ by $P_{\mathfrak{K}}$. The orthogonal complement of a subspace $\mathfrak{K} \subset \mathfrak{H}$ is denoted by $\mathfrak{K}^{\perp}$.

The Bose-Fock space and the Fermi-Fock space for some one-particle Hilbert space $\mathfrak{h}$ are denoted by $\mathfrak{F}_+(\mathfrak{h})$ and $\mathfrak{F}_-(\mathfrak{h})$ (see Appendix A.1). The Hilbert space of square-summable sequences of complex numbers is $\ell^2(\mathcal{V})$, where $\mathcal{V}$ is the index set of the sequence. For a vectors $f, g \in \mathbb{C}^d$, $d \in \mathbb{N}$, we sometimes write $f \cdot g = \langle f, g\rangle_{\mathbb{C}^d}$.

Linear operators The linear operators on $\mathfrak{H}$ are denoted by $\mathfrak{L}(\mathfrak{H})$, the bounded linear operators by $\mathfrak{B}(\mathfrak{H})$. Furthermore, $\mathfrak{L}_p(\mathfrak{H})$ with norm $\|\cdot\|_p$ are the Schatten class operators of order $p \in [1, \infty]$. In particular, $\mathfrak{L}_1(\mathfrak{H})$ with norm $\|\cdot\|_1$ are the trace class operators, $\mathfrak{L}_2(\mathfrak{H})$ with norm $\|\cdot\|_2$ are the Hilbert-Schmidt operators, and $\mathfrak{L}_\infty(\mathfrak{H})$ are the compact operators. The linear operators from $\mathfrak{H}$ to $\mathcal{H}$ are $\mathfrak{L}(\mathfrak{H}, \mathcal{H})$ and analogous notation is used for $\mathfrak{B}$ and $\mathfrak{L}_p$. The domain of an operator $A \in \mathfrak{L}(\mathfrak{H})$ is denoted by $\mathrm{dom}(A)$. The range of A is $\mathrm{ran}(A)$, the kernel is $\ker(A)$. If $A \in \mathfrak{L}_1(\mathfrak{H})$, its trace is denoted by $\mathrm{Tr}(A)$. The restriction of an operator A to the subspace $\mathfrak{K} \subset \mathfrak{H}$ is denoted by $A \restriction \mathfrak{K}$. The adjoint of A is A^* and its graph norm is $\|\cdot\|_A$. The strong, the weak, and the absolute Abelian limit are denoted by s-lim, w-lim, and |A|-lim, respectively. Here, $g \in \mathfrak{H}$ is the absolute Abelian limit of $g(t) \in \mathfrak{H}$, $t \in \mathbb{R}$, if and only if $\text{s-lim}_{\epsilon\to+0} \int_0^\infty \mathrm{d}t\, \epsilon e^{-\epsilon t}\|g(t) - g\|^2$ exists. The identity on a Hilbert space $\mathfrak{H}$ is denoted by $I_{\mathfrak{H}}$. In particular, we write $I_{el} = I_{\mathfrak{h}^{el}}$ and $I_{ph} = I_{\mathfrak{h}^{ph}}$. We often write $I = 1$ for the identity if no confusion is possible, i.e. for some $\zeta \in \mathbb{C}$ we write $\zeta\, I = \zeta$ in many cases. H and h, possibly with sub- or superscripts, always denote Hamiltonians, i.e. self-adjoint linear operators. We only consider Hamiltonians that are bounded from below. K, possibly with subscript, denotes a bounded self-adjoint linear operator, usually related to some Hamiltonian H by $K = (H + \theta)^{-N}$, $N \in \mathbb{N}$, with sufficiently large $\theta > 0$. Perturbations of the Hamiltonians, i.e. coupling operators or potentials, are denoted by V or v, possibly with subscript. For $V = V^*$, we denote its absolute value by $|V| = (V^*V)^{\frac{1}{2}}$ and its sign by $\mathrm{sgn}(V)$.

Second quantization For the convenience of the reader, the fundamentals of second quantization are summarized in Appendix A.1. The operators $a^*(f)$ and $a(g)$ for $f, g \in \mathfrak{h}$ are the usual creation and annihilation operators, respectively, on the bosonic Fock space $\mathfrak{F}_+(\mathfrak{h})$. For the fermionic case we write $b^*(f)$ respectively $b(g)$. If $\mathfrak{h}$ is one-dimensional, we drop the argument f respectively g. The second quantization of an operator A on $\mathfrak{h}$ is denoted by $\mathrm{d}\Gamma(A)$. The algebras generated by the canonical commutation relations and the canonical anti-commutation relations are denoted by $\mathcal{A}_+(\mathfrak{h})$ respectively $\mathcal{A}_-(\mathfrak{h})$.

Scattering theory For the convenience of the reader, a brief introduction into scattering theory is given in Appendix A.2. In a scattering system $\{H_0, H\}$, the unperturbed Hamiltonian is H_0, whereas H represents the interacting system. The wave operators are $W_\pm(H, H_0)$, and $W_\pm(\epsilon)$, $\epsilon > 0$, denotes the stationary pre-wave operator. Furthermore,

we have the scattering operator $S = W_+^*(H, H_0)W_-(H, H_0)$ and the transition operator $T = (2\pi i)^{-1}(1 - S)$.

Tensor products For two Hilbert spaces $\mathfrak{H}_1$, $\mathfrak{H}_2$, we write $\mathfrak{H}_1 \otimes \mathfrak{H}_2$ for the closure of the algebraic tensor product with respect to $\|f_1 \otimes f_2\|_{\mathfrak{H}_1\otimes\mathfrak{H}_2} = \|f_1\|_{\mathfrak{H}_1}\|f_2\|_{\mathfrak{H}_2}$. Similarly, let $A \in \mathfrak{L}(\mathfrak{H}_1)$, $B \in \mathfrak{L}(\mathfrak{H}_2)$. Then $A \otimes B$ denotes the closure of the linear operator given by linear extension of $(A \otimes B)(f_1 \otimes f_2) = Af_1 \otimes Bf_2$, $f_1 \in \mathrm{dom}(A)$, $f_2 \in \mathrm{dom}(B)$. The (anti-)symmetric tensor product is denoted by $\otimes_\pm$, cf. (A.1.1) in the Appendix.

L^p-spaces For a measure space $(\mathcal{O}, \Sigma, \mathfrak{m})$, the usual L^p space, $p \in [1, \infty]$, of $\mathfrak{m}$-a.e. defined functions with values in $\mathfrak{H}$ is denoted by $L^p(\mathcal{O}, \mathrm{d}\mathfrak{m}(\mu), \mathfrak{H})$. The μ in $\mathrm{d}\mathfrak{m}(\mu)$ indicates the subsequent label for the independent variable and "$\mathfrak{m}$-a.e." means for all $\mu \in \mathcal{O} \setminus \Xi$ for some set $\Xi \subset \mathcal{O}$ with $\mathfrak{m}(\Xi) = 0$. For the special case $\mathfrak{H} = \mathbb{C}$, we abbreviate $L^p(\mathcal{O}, \mathrm{d}\mathfrak{m}(\mu), \mathbb{C}) = L^p(\mathcal{O}, \mathrm{d}\mathfrak{m}(\mu))$. Also, if $\mathrm{d}\mathfrak{m}(\mu) = \mathrm{d}\mu\mathrm{Q}$ is the Lebesgue measure, we write $L^p(\mathcal{O}, \mathrm{d}\mu) = L^p(\mathcal{O})$. For $\Xi \subset \mathbb{R}$ we write $C_0^\infty(\Xi)$ for the smooth functions compactly supported on Ξ. The usual Sobolev space of l-times weakly differentiable L^p-functions with values in $\mathfrak{H}$ is $W^{l,p}(\Xi, \mathfrak{H})$. We write $W^{l,p}(\Xi)$ if $\mathfrak{H} = \mathbb{C}$. The Borel sets on $\mathbb{R}$ are denoted by $\mathcal{B}(\mathbb{R})$. Also, $\delta(\cdot)$ is the delta distribution and δ_{xy} is the Kronecker delta. The number of elements of an arbitrary set Ξ is $\mathrm{card}(\Xi) \in \mathbb{N}_0 \cup \{\infty\}$. The characteristic function of a set Ξ is denoted by χ_Ξ. For a measurable $\Xi \subset \mathbb{R}$, the Lebesgue measure of Ξ is denoted by $|\Xi|$. Let $r > 0$ and $\epsilon > 0$. A partition $\mathcal{J}_\epsilon^r$ for the interval $[-r, r)$ is a set of intervals $[r_n, r_{n+1})$, $0 \le n \le N$, such that $-r = r_0$, $r_n < r_{n+1}$, $r = r_N$, and $|\mathcal{J}_\epsilon^r| = \max_{1\le n\le N}(r_n - r_{n-1}) = \epsilon$.

Spectral measures For a self-adjoint operator H_0, its spectrum is $\sigma(H_0)$. The absolutely continuous, singular continuous, and pure point parts of the spectrum are denoted by $\sigma_{ac}(H_0)$, $\sigma_{sc}(H_0)$, and $\sigma_{pp}(H_0)$, respectively. If H_0 acts on $\mathfrak{H}$, the absolutely continuous, singular continuous, and pure point subspace are $\mathfrak{H}_{H_0}^{ac}$, $\mathfrak{H}_{H_0}^{sc}$, and $\mathfrak{H}_{H_0}^{pp}$. Furthermore, we write $P_{H_0}^j = P_{\mathfrak{H}_{H_0}^j}$ for $j \in \{ac, sc, pp\}$. The spectral measure of H_0 on $\mathcal{B}(\mathbb{R})$ is denoted by $E_{H_0}(\cdot)$, the absolutely continuous, singular continuous and pure point parts by $E_{H_0}^{ac}(\cdot)$, $E_{H_0}^{sc}(\cdot)$, and $E_{H_0}^{pp}(\cdot)$.

A spectral representation Φ of H on the direct integral $L^2(\mathbb{R}, \mathrm{d}\mathfrak{m}_H(\lambda), \mathfrak{H}_\lambda)$ is an isometric isomorphism $\Phi : \mathfrak{H} \to L^2(\mathbb{R}, \mathrm{d}\mathfrak{m}_H(\lambda), \mathfrak{H}_\lambda)$ such that $(\Phi Hf)(\lambda) = \lambda f(\lambda)$ for $\mathfrak{m}$-a.e. $\lambda \in \mathbb{R}$ and every $f \in \mathfrak{H}$. We denote spectral representations of H_0^{ac} and K_0^{ac} by Φ_{H_0} respectively Φ_{K_0}. We write $\Phi_{H_0} f = \widehat{f}$ and $\Phi_{K_0} f = \check{f}$. If X is an $\mathfrak{m}$-measurable function on $\mathbb{R}$ with values $X(\mu) \in \mathfrak{L}(\mathfrak{H}(\mu))$, the corresponding multiplication operator is denoted by $\mathcal{M}(X(\mu)) \in \mathfrak{L}(L^2(\mathbb{R}, \mathrm{d}\mathfrak{m}(\mu), \mathfrak{H}(\mu)))$, where μ indicates the independent variable, i.e. we define $(\mathcal{M}(X(\mu))\widehat{f})(\mu) = X(\mu)\widehat{f}(\mu)$ for every $\widehat{f} \in L^2(\mathbb{R}, \mathrm{d}\mathfrak{m}_H(\mu), \mathfrak{H}(\mu))$. We identify X and the induced multiplication operator $\mathcal{M}(X(\mu))$, i.e. we write $(X\widehat{f})(\mu) = (\mathcal{M}(X(\mu))\widehat{f})(\mu) = X(\mu)\widehat{f}(\mu)$.

Note that any operator $A \in \mathfrak{L}(\mathfrak{H})$ commuting with H_0 is mapped to a multiplication operator by a spectral representation of H_0, cf. Appendix A.2.5. We denote this multiplication operator by $(\Phi_{H_0} Af)(\lambda) = A(\lambda)\widehat{f}(\lambda)$ and $(\Phi_{K_0} Af)(\lambda) = \check{A}(\lambda)\check{f}(\lambda)$ if A commutes with H_0^{ac} respectively K_0^{ac}. In particular, the scattering matrix and the transition matrix are given by $S(\lambda)$ respectively $T(\lambda)$ for the scattering system $\{H_0, H\}$ and by $\check{S}(\lambda)$ respectively $\check{T}(\lambda)$ for the scattering system $\{K_0, K\}$.

Units We use units such that the reduced Planck constant $\hbar$, the elementary charge $\mathfrak{e}$, and the electric constant $\frac{1}{4\pi\epsilon_0}$ are equal to one. The electron mass satisfies $m_{el} = \frac{1}{2}$ and the dimensionless fine-structure constant $\alpha \approx \frac{1}{137}$ keeps its value.

2 Electron-photon interaction models

To be able to model a QD-LED, we need to model the emission of light by electrons. In this chapter we give a short presentation of the standard model of non-relativistic quantum electrodynamics, which describes the interaction of non-relativistic electrons with the electromagnetic field, i.e. with photons. Since this model is mathematically very difficult, we present two further electron-photon interaction models. They still capture essential features of the interaction, but are considerably more easy to handle. For those two models we derive Landauer-Büttiker formulae in Chapters 3 and 5.

2.1 The standard model of non-relativistic quantum electrodynamics

The standard model of non-relativistic quantum electrodynamics describes a fixed number of non-relativistic electrons interacting with a photon field. It is usually used to describe electrons bound to a nucleus in which excited electrons can emit photons to relax to the ground state. In particular, the speed of the electrons is supposed to be small with respect to the speed of light and the electron-positron pair creation is neglected. Our short presentation of the model is based on Bach et al. [5, 6] and Fröhlich et al. [45]. For a detailed exposition of the standard model, see Cohen-Tannoudji et al. [23].

Let N be the fixed number of electrons in the system we want to consider. The electron Hilbert space is the usual space $\mathfrak{h}^{el} = \left(L^2(\mathbb{R}^3, \mathrm{d}^3x, \mathbb{C}^2)\right)^{\otimes_- N}$ of anti-symmetric functions in $x = (x^{(1)}, \ldots, x^{(N)})$, where $x^{(n)}$ is the position of the n-th electron and $\mathbb{C}^2$ accounts for the spin of the electron. Note that we have to use the anti-symmetrized tensor product $\otimes_-$ since the electrons are fermions (see Appendix A.1). The single particle Hilbert space of the photons is $L^2(\mathbb{R}^3, \mathrm{d}^3k, \mathbb{C}^2)$, where k is the momentum of the photon and $\mathbb{C}^2$ accounts for the polarization of the photons. For a given non-zero photon momentum $k \in \mathbb{R}^3$, the transversal polarization vectors are denoted by $\{\varepsilon_-(k), \varepsilon_+(k)\}$ and satisfy $\varepsilon_\pm(k) \cdot k = 0$ and $\varepsilon_s(k) \cdot \varepsilon_{s'}(k) = \delta_{ss'}$, $s, s' \in \{-, +\}$. It follows that the full Hilbert space of the photons is given by the bosonic Fock space $\mathfrak{H}^{ph} = \mathfrak{F}_+\big(L^2(\mathbb{R}^3, \mathrm{d}^3k, \mathbb{C}^2)\big)$. The Hilbert space of the whole system is hence

$$\mathfrak{H} = \left(L^2(\mathbb{R}^3, \mathrm{d}^3x, \mathbb{C}^2)\right)^{\otimes_- N} \otimes \mathfrak{F}_+\big(L^2(\mathbb{R}^3, \mathrm{d}^3k, \mathbb{C}^2)\big) \cong \left(L^2(\mathbb{R}^3, \mathrm{d}^3x, \mathbb{C}^2 \otimes \mathfrak{H}^{ph})\right)^{\otimes_- N}.$$

The coupling of the electrons to the photon field is constructed via *minimal coupling*, which is achieved by subtracting the charge times the vector field from the momentum of the electron. The Hamiltonian of the electron-photon system is given by

$$H_{QED} = \sum_{n=1}^{N} \Big(-i\nabla_{x^{(n)}} - 2\sqrt{\pi\alpha^3} A_\kappa^{(n)} \Big)^2 + V_{el} + \mathrm{d}\Gamma(\omega), \tag{2.1}$$

where $x = (x^{(1)}, \dots x^{(N)})$ and $\omega = \mathcal{M}(\omega(k))$ with $\omega(k) = \|k\|$. Let us explain the components of the Hamiltonian. For $n \in \{1, 2, \dots, N\}$, the gradient $-i\nabla_{x^{(n)}}$ is the momentum operator of the n-th electron. $A_\kappa^{(n)}$ denotes the quantized vector potential of the transverse field in Coulomb gauge. It is a (3+3)-element vector with entries that are multiplication operators on $\left(L^2(\mathbb{R}^3, \mathrm{d}^3x, \mathbb{C}^2 \otimes \mathfrak{H}^{ph})\right)^{\otimes_- N}$ given by

$$(A_\kappa^{(n)}(x))_{j,s} = I_{\mathbb{C}^2} \otimes a^*(G_{j,s}(x^{(n)})) + I_{\mathbb{C}^2} \otimes a(G_{j,s}(x^{(n)})), \qquad j \in \{1,2,3\}, s \in \{-,+\},$$

with the usual bosonic creation and annihilation operators a^* and a (cf. Appendix A.1.2). Here, the functions $G_{j,s}(x^{(n)}) : \mathbb{R}^3 \to \mathbb{C}^3$ are given by

$$G_{j,s}(x^{(n)}, k) = \frac{\kappa(k)}{\pi\sqrt{2\omega(k)}} e^{-i\alpha k \cdot x^{(n)}} \big(\varepsilon_s(k)\big)_j. \tag{2.2}$$

The function $\omega(k) = \|k\|$ is the dispersion relation of the photon, $\kappa \in \mathcal{S}(\mathbb{R}^3)$ is an ultraviolet cutoff, and $\alpha \approx \frac{1}{137}$ is the fine-structure constant. In (2.1) the second quantized operator $\mathrm{d}\Gamma(\omega)$ is the energy of the free photons. The potential $V_{el}(x)$ is the sum of the Coulomb interaction and the static potential, i.e.

$$V_{el}(x) = \sum_{\substack{m,n=1 \\ m \neq n}}^{N} \frac{1}{|x^{(n)} - x^{(m)}|} + \sum_{n=1}^{N} v_{stat}(x^{(n)}).$$

The Hamiltonian H_{QED} is indeed self-adjoint on $\mathrm{dom}(H_{QED}) = \mathrm{dom}(-\Delta_x + \mathrm{d}\Gamma(\omega))$, where Δ_x is the Laplacian with respect to x. This is proven by Bach et al. [5] for sufficiently small coupling constant α. The proof of Hiroshima [51] makes no assumption on the value of α, but it only holds if the singularity in $G_{j,s}(x^{(n)})$ is of the order $|k|^{-\frac{1}{2}+\epsilon}$ for some small $\epsilon > 0$ and thus slightly milder than the physical case $|k|^{-\frac{1}{2}}$.

This infrared divergence of the order $|k|^{-\frac{1}{2}}$ is perhaps the most notable difficulty in the mathematical treatment of the model. In general, the spectral and scattering theory for H_{QED} is extremely challenging. The problem is linked to the fact that since $\omega(0) = 0$, i.e. the photons are massless, it is possible to have an infinite amount of photons with finite total energy. This is sometimes called a *soft photon cloud* [43, 68]. It implies that the eigenvalues of H_{QED} with $\alpha = 0$, i.e. without electron-photon interaction, are not separated from the absolutely continuous spectrum, whence standard perturbation theory fails.

Most papers concerned with the spectral theory of H_{QED} treat the fine-structure constant α as a small parameter and derive results valid for sufficiently small α without proving that the physical case $\alpha \approx \frac{1}{137}$ is actually covered by the results. We already mentioned that the proof of self-adjointness for H_{QED} of Bach et al. [5] used this approach. Bach et al. [6] proved that the spectrum of H_{QED} is purely absolutely continuous in the neighborhoods of the eigenvalues corresponding to excited eigenvalues of the electron Hamiltonian. Also, Bach et al. [3, 4] showed that H_{QED} has a ground state for small α, i.e. an eigenvalue at the bottom of its spectrum, and that the spectrum is absolutely continuous outside the neighborhoods of the eigenvalues of the electron Hamiltonian for small α. The excited states turn into resonances. Finally, Fröhlich

et al. [45] completed the spectral analysis by proving that the spectrum is absolutely continuous in a neighborhood of the ground state if α is small. This stepwise analysis of the spectral properties over one decade illustrates how mathematically challenging the standard model is.

Results in scattering theory are even more difficult to obtain. Most analysis is concerned with Rayleigh scattering, i.e. with incident photons being scattered at the bound electrons. In this setting, including an infrared cutoff, the existence of asymptotic electromagnetic fields has been proven in Fröhlich et al. [42], asymptotic completeness followed in Fröhlich et al. [44]. Since we want to calculate an electron current, the consideration of bound electrons is not sufficient for us. The model has to remain treatable if we connect the small quantum system to semi-infinite leads. A case of unbound electrons was considered in Fröhlich et al. [43] and asymptotic completeness was proven. But the paper did consider only the case of free electrons. Since we want to consider the transition of electrons through a small quantum system, this is not a suitable setting for us.

Considering the mathematical complexity of the full physical model, we do not aim at deriving a current formula for a QD-LED based on the standard model. In the following sections we introduce two simplified toy models, the Pauli-Fierz models and the Jaynes-Cummings model, that are based on physical models and each of which contains some essential features that are of interest to us. As a general simplification, we restrict the interaction of the electrons and the photons to the small quantum system. This allows us to use the existing theory on models with localized electrons. In this thesis we use a Pauli-Fierz model and the Jaynes-Cummings model to construct models of a QD-LED. Namely, we present a Jaynes-Cummings QD-LED in Chapter 3 and a Pauli-Fierz QD-LED in Chapter 5.

2.2 The Pauli-Fierz model

The Pauli-Fierz model is a simplified model of quantum electrodynamics with a localized interaction. The terminology is not fully consistent in the literature. In the present work we follow Dereziński and Gérard [35] and Dereziński and Jaksic [36]. Strictly speaking, Pauli-Fierz models are rather a class of models with common properties than one single model. They are inspired by the the works of Pauli and Fierz [66]. The general idea is that a small quantum system (e.g. an atom, a quantum dot) is coupled to the electromagnetic field. Smallness means that the electron Hamiltonian has compact resolvent. In the case of an atom, this is achieved by cutting off energies above the ionization threshold, i.e. by projecting onto the space spanned by the eigenvectors. Since the restrictions on the form factor of the interaction between the quantum system and the field are mild, a wide range of models can be cast in the Pauli-Fierz form. In particular, three-dimensional models with polarized fields are possible.

In our case the small quantum system is a one-dimensional electron in a potential well. It interacts with a scalar field through an interaction that is derived from the standard model of Section 2.1.

2.2.1 Mathematical model

We call the small quantum system the *electron system* and the electromagnetic field the *photon field*, even though we have scalar field particles, to keep the connection to the QD-LED that we want to model. The electron Hilbert space of the quantum system, indexed by S, is

$$\mathfrak{h}_S^{el} = L^2((a,b), \mathrm{d}x)$$

with Hamiltonian

$$h_S^{el} = -\tfrac{\mathrm{d}^2}{\mathrm{d}x^2} + v(x)$$

for some bounded measurable potential $v : (a,b) \to \mathbb{R}$. We choose homogeneous Dirichlet boundary conditions for the second derivative, i.e.

$$\mathrm{dom}(h_S^{el}) = \{f \in W^{2,2}((a,b)) \,|\, f(a) = f(b) = 0\}.$$

It is well known that this Hamiltonian is self-adjoint and has compact resolvent [31]. The Hilbert space of a single photon is $\mathfrak{h}_1^{ph} = L^2(\mathbb{R}, \mathrm{d}k)$, where k is the photon energy. The full photon Hilbert space is hence

$$\mathfrak{H}^{ph} = \mathfrak{F}_+\big(L^2(\mathbb{R}, \mathrm{d}k)\big).$$

Let $\omega : \mathbb{R} \to \mathbb{R}_+ \cup \{0\}$, $\omega(k) = |k|$ be the dispersion relation of the photons. Note that although we have a scalar field, the dispersion relation is 'photonic', i.e. linear in the photon momentum . The free photon Hamiltonian is given by

$$H^{ph} = \mathrm{d}\Gamma\big(\mathcal{M}(\omega(k))\big).$$

The full Hilbert space of the system is

$$\mathfrak{H} = \mathfrak{h}_S^{el} \otimes \mathfrak{H}^{ph} = L^2\big((a,b), \mathrm{d}x, \mathfrak{F}_+(\mathfrak{h}_1^{ph})\big).$$

The interaction in the Pauli-Fierz model is given by a form factor $G \in \mathfrak{B}(\mathfrak{h}^{el}, \mathfrak{h}^{el} \otimes \mathfrak{h}_1^{ph})$ (cf. Appendix A.1). The interaction Hamiltonian is

$$V_{int} = a^*(G) + a(G). \tag{2.3}$$

Obviously, there is much freedom in the choice of the form factor and the specific choice is responsible for the physics of the model. We choose a model that was introduced in a similar form by Pauli and Fierz [66] and gave the class of Pauli-Fierz models its name (see also [35, 36]). Let $G = \mathcal{M}\big(G(x,k)\big)$ with

$$G(x,k) = e^{ikx}\omega(k)^{-\frac{1}{2}}\kappa(k),$$

where $\kappa \in C_0^\infty(\mathbb{R}_+)$ serves as an infrared cutoff and an ultraviolet cutoff, and $\omega(k) = |k|$ is the dispersion relation of the photons. This model is also sometimes referred to as the *Nelson model*, cf. Nelson [64], although some authors reserve this term for free electrons on $\mathbb{R}$ with the interaction extended to the whole real line. Note that the form factor is very similar to the interaction in the standard model of non-relativistic quantum

electrodynamics (2.2). The total Pauli-Fierz Hamiltonian is given by

$$H_{PF} = h_S^{el} \otimes I_{ph} + I_{\mathfrak{h}_S^{el}} \otimes H^{ph} + \tau_{int} V_{int},$$

where $\tau_{int} > 0$ is a coupling constant. Hiroshima [51] and Georgescu et al. [49] proved that H_{PF} is self-adjoint on $\mathrm{dom}(H_{PF}) = \mathrm{dom}(h_S^{el} \otimes I_{ph}) \cap \mathrm{dom}(I_{\mathfrak{h}_S^{el}} \otimes H^{ph})$. From Georgescu et al. [49], we also get that the essential spectrum of H_{PF} is given by $\sigma_{ess}(H_{PF}) = [\inf \sigma(H_{PF}), +\infty)$. The singular continuous spectrum is empty and the pure point spectrum is locally finite, i.e. $\mathrm{Tr}(E^{pp}_{H_{PF}}(\Xi)) < \infty$ for all bounded intervals $\Xi \subset \mathbb{R}$. Further results on the spectral properties can be found in [40].

It is very natural for the model to contain an ultraviolet cutoff since we treat a non-relativistic electron. In contrast, the infrared regularization is introduced for convenience since the infrared divergency in the full model is rather hard to handle. Our main interest lies in the formulation of a QD-LED model for which the Pauli-Fierz model is a starting point, and we do not want to get hindered by the subtleties which arise through the infrared divergencies. This is a reasonable simplification if the infrared cutoff is small with respect to the eigenvalues of h_S^{el}. Note that the infrared regularization in the interaction is similar to the introduction of a rest mass for the photons, a key point being that in both situations it is not possible to create infinitely many low-energy photons with finite total energy. It is not the same, however, since a non-zero photon rest mass implies a spectral gap between the lowest eigenvalue and the beginning of the absolutely continuous spectrum in the spectrum of the non-interacting Hamiltonian $h_S^{el} \otimes I_{ph} + I_{\mathfrak{h}_S^{el}} \otimes H^{ph}$.

2.2.2 The 1-photon Pauli-Fierz model

A further simplification of the Pauli-Fierz model, which is not uncommon in the literature, is to introduce a particle number cutoff for the photons. This idea goes back to Friedrichs [41] and was also used by Hübner and Spohn [52]. We want to restrict ourselves to the case of at most one photon, a concept also used by Gérard et al. [50] and Galtbayar et al. [46], among others. Hence, we introduce the subspace of at most one photon. It is the sum of the no-photon space $\mathbb{C}\Omega \subset \mathfrak{F}_+(L^2(\mathbb{R}, \mathrm{d}k))$, where $\Omega = (1, 0, 0, \ldots) \in \mathfrak{F}_+(L^2(\mathbb{R}, \mathrm{d}k))$ is the vacuum vector, and the one-photon space $L^2(\mathbb{R}, \mathrm{d}k) \subset \mathfrak{F}_+(L^2(\mathbb{R}, \mathrm{d}k))$. Thus,

$$\mathfrak{h}^{ph} = \mathbb{C}\Omega \oplus L^2(\mathbb{R}, \mathrm{d}k) \subset \mathfrak{F}_+(L^2(\mathbb{R}, \mathrm{d}k)) = \mathfrak{H}^{ph}$$

is the space of at most one photon. The total Hilbert space of the quantum system is then

$$\mathfrak{H}_S = \mathfrak{h}_S^{el} \otimes \mathfrak{h}^{ph}.$$

Note that $H^{ph}\Omega = 0$ and $(H^{ph} f_1^{ph})(k) = \omega(k) f(k)$, $f_1^{ph} \in L^2(\mathbb{R}, \mathrm{d}k)$, whence

$$h^{ph} = H^{ph} \restriction \mathfrak{h}^{ph} = \begin{pmatrix} 0 & 0 \\ 0 & \mathcal{M}(\omega(k)) \end{pmatrix}$$

with

$$\mathrm{dom}(h^{ph}) = \Big\{(f_0^{ph}, f_1^{ph}) \in \mathfrak{h}^{ph} \,\Big|\, \int_{\mathbb{R}} \mathrm{d}k\, |\omega(k) f_1^{ph})(k)|^2 < \infty\Big\}.$$

The annihilation operator satisfies

$$a(G(x))\Omega = 0, \qquad a(G(x))f_1^{ph} = \langle G(x), f_1^{ph}\rangle, \qquad f_1^{ph} \in L^2(\mathbb{R}, \mathrm{d}k).$$

Hence, from the restriction of (2.3) to the one-photon subspace $\mathfrak{H}_S$, we obtain

$$V_{ph,1} = \begin{pmatrix} 0 & \mathcal{M}(\langle G(x)|) \\ \mathcal{M}(|G(x)\rangle) & 0 \end{pmatrix}$$

on $L^2\big((a,b)\mathrm{d}x\big) \oplus L^2\big((a,b)\times\mathbb{R}, \mathrm{d}x\times\mathrm{d}k\big)$ for the electron-photon interaction, where

$$\langle G(x)| : \mathfrak{h}^{ph} \to \mathbb{C}, \qquad (\langle G(x)|f_1^{ph})(k) = \int_{\mathbb{R}} \mathrm{d}k\, \overline{G(x,k)} f_1^{ph}(k),$$

for $x \in (a,b)$ and $|G(x)\rangle = \langle G(x)|^*$. The total Hamiltonian is

$$H_{PF,1} = \begin{pmatrix} -\Delta_x + v & \tau_{int}\langle G| \\ \tau_{int}|G\rangle & -\Delta_x + v + \omega \end{pmatrix}$$

on $L^2\big((a,b),\mathrm{d}x\big) \oplus L^2\big((a,b)\times\mathbb{R}, \mathrm{d}x\times\mathrm{d}k\big)$. Recall that we choose homogeneous Dirichlet boundary conditions for $-\Delta_x$.

This is the model we use in Chapter 5 to model a QD-LED in which arbitrary photon energies are possible. This continuous photon energy causes some mathematical difficulties. In a model of a QD-LED, we have to contact the quantum dot with leads, and we will see that this coupling of the leads to the quantum dot is not relatively trace class in the Pauli-Fierz model. This motivates us to prove a Landauer-Büttiker formula in Chapter 5 that is more general than what can be found in the literature and that is adapted to this situation.

2.3 The Jaynes-Cummings model

The Jaynes-Cummings model is mathematically simpler than the Pauli-Fierz models. It describes a two-level atom interacting with photons of a fixed frequency. This restriction to a single photon energy has the advantage that the model remains tractable even with arbitrary photon numbers. The model was introduced by Jaynes and Cummings [53] to compare the effects of a quantized field model to the results for a semiclassical theory concerning spontaneous emission rates. Since then, it has been used for a variety of physical phenomena, e.g. stimulated emission, anti-bunching, and quantum correlation [1, 14, 16, 29, 47]. The model is of particular interest because it is a simple model that still contains effects of pure quantum nature, like periodic collapse and revival of the occupancy of the excited state [37], also called Rabi oscillation. Generalizations of the Jaynes-Cummings model have been made, including damping effects [48], multiple atoms [57], and multiple energy levels [17, 56]. An overview of the applications and generalizations of the Jaynes-Cummings model can be found in [76].

The first modeling assumption made in the Jaynes-Cummings model is to model matter as a simple two level system, representing an atom or molecule with its ground state and the first excited state. This approach is particularly suited to describe quantum dots, which were not yet discovered when the Jaynes-Cummings model was first proposed (see [39, 70] for early papers on quantum dots). The two-level system is then supposed to reside in a cavity that has a discrete set of resonant frequencies, called *modes* of the electromagnetic field. The cavity is tuned such that one mode matches the energy difference between the two levels of the system. Thus, the two-level system effectively interacts only with a single mode of the electromagnetic field. This interaction is given by the coupling of the dipole moment of the two-level system to the field. A simplification of the model called *rotating wave approximation*, which is valid for well-tuned cavities, makes the model explicitely diagonalizable. This makes the model quite interesting for a rigorous treatment of electron-photon interaction effects. For a physical discussion of the model, see Cohen-Tannoudji et al. [24, Ch. 6]. In this thesis we use the model to describe a QD-LED, i.e. the two-level system describes an electron in a quantum dot.

2.3.1 Mathematical model

The electron Hilbert space of the two-level quantum system, indexed by S, is

$$\mathfrak{h}_S^{el} = \mathbb{C}^2.$$

Although we formulate an abstract model, we call the two-level system *electron system* and think of it as an electron in a two-level quantum dot. Let h_S^{el} be the self-adjoint Hamiltonian of the electron system with eigenvectors e_0 and e_1 for eigenvalues λ_0 and λ_1, respectively, with $\lambda_1 > \lambda_0$. We can use the identification $\mathfrak{h}_S^{el} = \mathbb{C}^2 = \mathfrak{F}_-(\mathbb{C}e_1)$, where $\Omega = (1,0) = e_0$ and $e_1 = (0,1)$, to write this in the Fock space setting, which is a convenient language for the model (cf. Appendix A.1, Example A.1.1). Since $\mathbb{C}e_1$ is one-dimensional, we have only one annihilation operator $b(e_1)$. We abbreviate $b \equiv b(e_1)$. Then b^* and b create and annihilate excitations, respectively, and we can write the quantum dot Hamiltonian as $h_S^{el} = (\lambda_1 - \lambda_0)b^*b + \lambda_0$. Without loss of generality we choose $\lambda_0 = 0$ and set $\lambda_1 = \omega_0$, which gives us

$$h_S^{el} = \omega_0 b^* b.$$

The electron system interacts only with a single mode of the electromagnetic field, whence the photon Hilbert space is

$$\mathfrak{h}^{ph} = \mathfrak{F}_+(\mathbb{C})$$

with annihilation and creation operators a and a^*. Again, it is an abstract model in which a^* creates bosonic particles all in the same single particle state. Keeping the application in mind, we call the particles *photons*. We can identify $\mathfrak{h}^{ph} = \ell^2(\mathbb{N}_0)$ and in this sense

$$\mathrm{dom}(a) = \mathrm{dom}(a^*) = \mathrm{dom}(\mathfrak{N}_+^{\frac{1}{2}}) = \Big\{(k_0, k_1, k_2, \ldots) \in \ell^2(\mathbb{N}_0) \,\Big|\, \sum_n n|k_n|^2 < \infty\Big\},$$

where $\mathfrak{N}_+ = a^*a = \mathrm{d}\Gamma(I_{\mathbb{C}})$ is the photon number operator. Let ω be the fixed frequency of the photons. Then the Hamiltonian of the photon field is

$$h^{ph} = \omega\, a^*a = \omega\, \mathrm{d}\Gamma(I_{\mathbb{C}}). \tag{2.4}$$

It is self-adjoint on the domain $\mathrm{dom}(\mathfrak{N}_+)$. The full Hilbert space of the system is

$$\mathfrak{H}_S = \mathfrak{h}_S^{el} \otimes \mathfrak{h}^{ph}.$$

The interaction of the electron with the photons is derived from the coupling of the dipole moment of the electron to the electromagnetic field [24, Sec. VI.B.3]). We have

$$\tilde{V}_{int} = (b^* + b) \otimes (a + a^*).$$

This interaction decomposes into $\tilde{V}_{int} = V_{int} + V_{int}^{cr}$ with

$$V_{int} = b^* \otimes a + b \otimes a^*, \qquad V_{int}^{cr} = b^* \otimes a^* + b \otimes a.$$

To see that we can neglect the term V_{int}^{cr}, we consider the free evolution of the interaction energy driven by $H_0 = h_S^{el} \otimes I_{ph} + I_{\mathfrak{h}_S^{el}} \otimes h^{ph}$. Let $\{\Upsilon_n\}_{n\in\mathbb{N}_0}$ be the canonical basis of $\mathfrak{h}^{ph} = \ell^2(\mathbb{N}_0)$. Note that $e^{itH_0}(e_m \otimes \Upsilon_n) = e^{it(m\omega_0 + n\omega)} e_m \otimes \Upsilon_n$ for $m \in \{0, 1\}$, $n \in \mathbb{N}_0$. This implies

$$e^{itH_0} V_{int} e^{-itH_0} = e^{it(\omega_0 - \omega)} b^* \otimes a + e^{-it(\omega_0 - \omega)} b \otimes a^*$$

and

$$e^{itH_0} V_{int}^{cr} e^{-itH_0} = e^{it(\omega_0 + \omega)} b^* \otimes a^* + e^{-it(\omega_0 + \omega)} b \otimes a.$$

Note that the factor $e^{\pm it(\omega_0+\omega)}$ is oscillating much faster than $e^{\pm it(\omega_0-\omega)}$. The *rotating wave approximation* states that we can neglect the so-called *counter-rotating* term V_{int}^{cr}. There are no precise mathematical statements about the validity of this approximation, but good agreement with experiments is obtained if the cavity is well-tuned to the energy gap of the electron system, i.e. $\omega_0 - \omega \ll \min(\omega_0, \omega)$, in a weak-coupling regime [16]. The final model hence reads

$$H_{JC} = \omega_0 (b^*b \otimes I_{ph}) + \omega (I_{\mathfrak{h}_S^{el}} \otimes a^*a) + \tau_{int} (b^* \otimes a + b \otimes a^*)$$

with some coupling constant $\tau_{int} > 0$. Note that the interaction term $b^* \otimes a$ corresponds to an electron jumping from the ground state to the excited state by absorbing a photon. Vice versa, $b \otimes a^*$ corresponds to the relaxation to the ground state by emitting a photon.

Lemma 2.3.1. *The Jaynes-Cummings Hamiltonian H_{JC} is a bounded from below self-adjoint operator on the domain* $\mathrm{dom}(H_{JC}) = \mathrm{dom}(I_{\mathfrak{h}_S^{el}} \otimes h^{ph})$.

Proof. Let $c \geq 2$. Then

$$\|a\Upsilon_n\|^2 \leq \|a^*\Upsilon_n\|^2 = n + 1 \leq c^{-1}n^2 + c,$$

for $n \in \mathbb{N}_0$. Consider elements $f \in \mathfrak{h}_S^{el} \otimes \mathfrak{h}^{ph} \cap \mathrm{dom}(I_{\mathfrak{h}_S^{el}} \otimes h^{ph})$ with

$$f = \sum_{j,l=1}^{N} \beta_{jl}\, e_{m_j} \otimes \Upsilon_{n_l}, \quad m_j \in \{0, \ldots, d-1\}, \quad n_l \in \mathbb{N}_0, \quad N \in \mathbb{N},$$

which are dense in $\mathfrak{H}_S$. Then $\|f\|^2 = \sum_{j,l=1}^{N} |\beta_{jl}|^2$ and $\|(I_{\mathfrak{h}_S^{el}} \otimes a^*a)f\|^2 = \sum_{j,l=1}^{N} |\beta_{jl}|^2 n_l^2$. We obtain

$$\begin{aligned}\|(b^* \otimes a)f\|^2 &\leq \sum_{j,l=1}^{N} |\beta_{jl}|^2 \|b^* e_{m_j}\|^2 \, \|a\Upsilon_{n_l}\|^2 \\ &\leq \sum_{j,l=1}^{N} |\beta_{jl}|^2 (c^{-1} n_l^2 + c) \\ &= c^{-1} \|(I_{\mathfrak{h}_S^{el}} \otimes a^*a)f\|^2 + c\|f\|^2\end{aligned}$$

Similarly,

$$\|(b \otimes a^*)f\|^2 \leq 2c^{-1} \|(I_{\mathfrak{h}_S^{el}} \otimes a^*a)f\|^2 + 2c\,\|f\|^2.$$

We may choose c arbitrarily large, whence we obtain that V_{int} is dominated by H^{ph} with relative bound zero. Since $h_S^{el} \otimes I_{ph}$ is self-adjoint and bounded and $I_{\mathfrak{h}_S^{el}} \otimes h^{ph}$ is self-adjoint and bounded from below, it follows that $H_{JC} = h_S^{el} \otimes I_{ph} + I_{\mathfrak{h}_S^{el}} \otimes h^{ph} + \tau_{int} V_{int}$ is a bounded from below self-adjoint operator on the domain $\mathrm{dom}(H_{JC}) = \mathrm{dom}(I_{\mathfrak{h}_S^{el}} \otimes h^{ph})$ for any $\tau_{int} > 0$ by [55, Thm. V.4.1]. □

2.3.2 Spectral properties

One nice property of the Jaynes-Cummings model is that it can be explicitly diagonalized. Recall the anti-commutation relations $b^*b = 1 - bb^*$ and the Pauli principle $b^*b^* = bb = 0$, cf. Appendix A.1. We obtain

$$\tau_{int}^{-1}[H_{JC}, b^*b \otimes I_{ph}] = (b^*b^*b - b^*bb^*) \otimes a + (bb^*b - b^*bb) \otimes a^* = -b^* \otimes a + b \otimes a^*. \quad (2.5)$$

The commutation relations $aa^* - a^*a = 1$ give us

$$\tau_{int}^{-1}[H_{JC}, I_{\mathfrak{h}_S^{el}} \otimes a^*a] = b^* \otimes (aa^*a - a^*aa) + b \otimes (a^*a^*a - a^*aa^*) = b^* \otimes a - b \otimes a^*. \quad (2.6)$$

Adding these two relations shows that the Jaynes-Cummings Hamiltonian H_{JC} commutes with the number operator $\mathfrak{N}_{JC} = b^*b \otimes I_{ph} + I_{\mathfrak{h}_S^{el}} \otimes a^*a$. Hence, it is reduced by the eigenspaces of the number operator. These eigenspaces are

$$\mathfrak{H}_{JC}^{(n)} = \mathrm{span}\{e_0 \otimes \Upsilon_n, e_1 \otimes \Upsilon_{n-1}\}, \qquad \mathfrak{H}_{JC}^{(0)} = \mathrm{span}\{e_0 \otimes \Upsilon_0\}, \qquad n \geq 1.$$

We get

$$H_{JC} = \bigoplus_{n \in \mathbb{N}_0} H_{JC}^{(n)}, \qquad H_{JC}^{(0)} = 0, \qquad H_{JC}^{(n)} = \begin{pmatrix} n\omega & \tau_{int}\sqrt{n} \\ \tau_{int}\sqrt{n} & \omega_0 + (n-1)\omega \end{pmatrix}, \qquad n \geq 1.$$

The eigenvalues $\lambda_{JC}^{\pm}(n)$ of $H_{JC}^{(n)}$, $n \geq 1$, are the solutions of

$$(n\omega - \lambda)(\omega_0 + (n-1)\omega - \lambda) - \tau_{int}^2 n = 0.$$

We obtain

$$\sigma(H_{JC}) = \sigma_{pp}(H_{JC}) = \left\{ n\omega + \tfrac{1}{2}(\omega_0 - \omega) \pm \sqrt{\tfrac{1}{4}(\omega_0 - \omega)^2 + \tau_{int}^2 n} \;\middle|\; n \in \mathbb{N} \right\} \cup \{0\}.$$

For the special case of a perfectly tuned cavity, i.e $\omega_0 = \omega$, we have

$$\sigma(H_{JC}) = \sigma_{pp}(H_{JC}) = \{ n\omega \pm \tau_{int}\sqrt{n} \mid n \in \mathbb{N} \} \cup \{0\}.$$

The eigenvectors can also be computed easily. Of course, with this decomposition we can also explicitly compute the resolvent $(H_{JC} - \zeta)^{-1}$, $\zeta \in \mathbb{C} \setminus \sigma(H_{JC})$. Thus, we have a complete understanding of the Jaynes-Cummings Hamiltonian H_{JC}.

2.3.3 Generalization of the Jaynes-Cummings model

It is quite straightforward to generalize the Jaynes-Cummings model to a system with $d \geq 2$ energy levels with constant energy gap ω_0 [17, 56]. In this case $\mathfrak{h}_S^{el} = \mathbb{C}^d$ is not written as a Fock space with creation and annihilation operators. However, we introduce the so-called *ladder operators* b^* and b. They are very similar and play essentially the same role. Let $\{e_0, \ldots, e_{d-1}\}$ be an orthonormal basis of $\mathbb{C}^d$ describing the energy levels of the quantum dot, i.e. $h_S^{el} e_m = m\omega_0\, e_m$. Then we define $b : \mathbb{C}^d \to \mathbb{C}^d$ and $b^* : \mathbb{C}^d \to \mathbb{C}^d$ by

$$b\, e_m = \sqrt{m}\, e_{m-1}, \qquad be_0 = 0, \qquad b^* e_{m-1} = \sqrt{m}\, e_m, \qquad b^* e_{d-1} = 0, \tag{2.7}$$

for $1 \leq m \leq d-1$. We obtain

$$\omega_0 b^* b\, e_m = m\omega_0\, e_m = h_S^{el} e_m.$$

The photon Hilbert space $\mathfrak{h}^{ph} = \mathfrak{F}_+(\mathbb{C}) = \ell^2(\mathbb{C})$ and the photon Hamiltonian $h^{ph} = \omega\, a^* a$ on $\mathrm{dom}(h^{ph}) = \mathrm{dom}(\mathfrak{N}_+)$ are the same as in the original Jaynes-Cummings model, where ω is again the resonance frequency of the cavity. Hence, we get the new total Hilbert space

$$\mathfrak{H}_S = \mathfrak{h}_S^{el} \otimes \mathfrak{h}^{ph} = \mathbb{C}^d \otimes \ell^2(\mathbb{C}).$$

The electron-photon interaction of the generalized model is also formally the same. We only replace the creation and annihilation operators by the ladder operators (2.7) and obtain

$$V_{int} = b^* \otimes a + b \otimes a^*.$$

Again, the terms reflect that an electron jumps to the next higher/lower energy level upon absorption/emission of a photon. As a result, the Hamiltonian of the generalized Jaynes-Cummings model with d energy levels is formally unchanged. Namely,

$$H_{GJC} = h_S^{el} \otimes I_{ph} + I_{\mathfrak{h}_S^{el}} \otimes h^{ph} + \tau_{int} V_{int},$$

for some coupling constant $\tau_{int} > 0$. It is also self-adjoint on the domain $\mathrm{dom}(I_{\mathfrak{h}_S^{el}} \otimes h^{ph})$. The diagonalization procedure of the previous section still applies for this generalized model. This is not immediately obvious since the ladder operators are no creation/annihilation operators and we do not have the canonical anti-commutation relations, which we used to show that $[V_{int}, \mathfrak{N}_{JC}] = 0$. However, direct calculations give us

$$bb^* e_{d-1} = 0, \qquad bb^* e_m = b\sqrt{m+1}\, e_{m+1} = (m+1)e_m, \qquad 0 \leq m < d-1.$$

Together with $b^*b\, e_m = m e_m$, this gives us

$$(b^*b - bb^*)e_{d-1} = (d-1)e_{d-1}, \qquad (b^*b - bb^*)e_m = -e_m, \qquad 0 \leq m < d-1.$$

Thus,

$$(b^*b^*b - b^*bb^*)e_m = \left\{ \begin{array}{cc} -\sqrt{m+1}\, e_{m+1} & \text{for} \quad 0 \leq m < d-1 \\ 0 & \text{for} \quad m = d-1 \end{array} \right\} = -b^* e_m$$

and

$$(bb^*b - b^*bb)e_m = \left\{ \begin{array}{cc} \sqrt{m}\, e_{m-1} & \text{for} \quad 1 \leq m \leq d-1 \\ 0 & \text{for} \quad m = 0 \end{array} \right\} = b\, e_m.$$

Now we can proceed as in (2.5) and (2.6) to show that $[V_{int}, \mathfrak{N}_{GJC}] = 0$ also for the generalized Jaynes-Cummings model, where $\mathfrak{N}_{GJC} = b^*b \otimes I_{ph} + I_{\mathfrak{h}_S^{el}} \otimes a^*a$ using the ladder operators. The eigenspace of $\mathfrak{N}_{GJC}$ for the eigenvalue $n \in \mathbb{N}_0$ is

$$\mathfrak{H}_{GJC}^{(n)} = \mathrm{span}\{e_m \otimes \Upsilon_{n-m} \,|\, 0 \leq m \leq d-1,\, n-m \geq 0\}.$$

It follows that $\sigma(H_{GJC}) = \sigma_{pp}(H_{GJC})$ and

$$H_{GJC} = \bigoplus_{n \in \mathbb{N}_0} H_{GJC}^{(n)},$$

where $H_{GJC}^{(n)}$ as operator on $\mathfrak{H}_{GJC}^{(n)}$ is at most a $d \times d$-matrix, whence the numerical calculation of the eigenvalues is straightforward.

3 The Landauer-Büttiker formula for a quantum dot LED

As mentioned in the introductory Chapter 1, the main goal of this thesis is the derivation of a formula for the electric current and the light production in a QD-LED. Our novel approach to achieve this goal is to cast this problem into the framework of the Landauer-Büttiker formalism.

The first goal of this chapter is to prove the Landauer-Büttiker formula for a quite general class of scattering systems. The second goal is the construction of a simple model of a quantum dot LED based on the Jaynes-Cummings model of Section 2.3 that allows us to apply the Landauer-Büttiker formalism to obtain formulae for the current and the light production. This usage of the Landauer-Büttiker formula beyond quasi-free electron systems is a novelty and significantly simplifies the calculation of fluxes in a QD-LED.

3.1 The abstract Landauer-Büttiker formula

The Landauer-Büttiker formula does not only apply to the simple setting of two leads contacted to a quantum system that we sketched in the introduction of this thesis. In fact, one can formulate an abstract Landauer-Büttiker formula that holds for any scattering system $\{H_0, H\}$ satisfying certain conditions, cf. Theorem 3.1.2. Also, it is not restricted to the electric current. Similar formulae can be derived for a large class of observables, including the energy flux and the entropy flux. A first proof of such an abstract Landauer-Büttiker formula was given by Nenciu [65]. Aschbacher et al. [2] established the formula under much weaker conditions on $\{H_0, H\}$. Our requirements on $\{H_0, H\}$ are similar to those of [2]. However, our definition of the flux is somewhat different in the sense that the regularization is achieved without a limiting procedure, cf. Definition 3.1.1. In principle, the proof of Aschbacher et al. [2] uses stationary scattering as we do in our proof. However, the presentation is very abstract and relies heavily on results that can be found in [80]. Since we use a rather explicit spectral representation, cf. Lemma 3.1.4, and our proof uses only well-known fundamentals of stationary scattering theory, it is very transparent. We think that this improves the understanding of the Landauer-Büttiker formula. Additionally, the representation of the transition matrix that we derive in Proposition 3.1.6 can be used to obtain an even more explicit formula of the transition matrix using boundary triplets, cf. Chapter 4. Finally, the idea of the proof and the basic tools can also be used to prove the more general Landauer-Büttiker formula for multiplication operators of Chapter 5.

3.1.1 The non-equilibrium steady state and the density operator

When we talk about a proof of the Landauer-Büttiker formula, this means that we want to derive the formula from the general principles of quantum mechanics. The essentials of second quantization, e.g. Fock spaces, quasi-free states, and the definition of $\mathrm{d}\Gamma$, can be found in Appendix A.1. In the following we illustrate this derivation using the example of the electric current in a system of two leads contacted to a quantum system given by the scattering system $\{h_0^{el}, h^{el}\}$. This derivation immediately generalizes to an abstract scattering system $\{H_0, H\}$.

We start with a many electron system represented on the Fock space $\mathfrak{F}_-(\mathfrak{h}^{el})$, where $\mathfrak{h}^{el}$ is the single-electron Hilbert space. In the Landauer-Büttiker framework, we assume that the electrons do not interact with each other. This implies that the Hamiltonian of the system is given by $\mathrm{d}\Gamma(h^{el})$, where h^{el} is the single-electron Hamiltonian. Thus, the evolution $\mathfrak{t}_t$ on the CAR-algebra $\mathcal{A}_-(\mathfrak{h}^{el})$ given by

$$\mathfrak{t}_t : \mathcal{A}_-(\mathfrak{h}^{el}) \to \mathcal{A}_-(\mathfrak{h}^{el}), \qquad A \mapsto e^{it\mathrm{d}\Gamma(h^{el})} A\, e^{-it\mathrm{d}\Gamma(h^{el})},$$

is also quasi-free for every $t \in \mathbb{R}$, i.e. if the initial state ϖ_0 is quasi-free, the states $\varpi_t = \varpi \circ \mathfrak{t}_t$ are also quasi-free for every $t \in \mathbb{R}$ [34]. A crucial point in the Landauer-Büttiker framework is that a quasi-free state ϖ_0 can be described by a density operator ρ_0^{el} on the single-particle space $\mathfrak{h}^{el}$ using the relation $\varpi(a^*(f)a(g)) = \langle g, \rho_0^{el} f\rangle_{\mathfrak{h}^{el}}$ for $f, g \in \mathfrak{h}^{el}$. Thus, we avoid the complicated Fock space and reduce everything to the original single-particle space. We want to emphasize that it is the assumption that electrons do not interact with eachother that gives us the quasi-free evolution, which in turn lets us describe the state with a density operator on the single-particle space. For a trace class operator $v_{el} \in \mathfrak{L}_1(\mathfrak{h}^{el})$, we even have the simple formula

$$\varpi_0(\mathrm{d}\Gamma(v_{el})) = \mathrm{Tr}_{\mathfrak{h}^{el}}(\rho_0^{el} v_{el}),$$

cf. Equation (A.1.9) in the appendix. If ρ_0^{el} is the single-particle density operator of ϖ_0, the single-particle density operator of ϖ_t is given by $\rho^{el}(t) = e^{-ith^{el}} \rho_0 e^{ith^{el}}$ for $t \in \mathbb{R}$, cf. Lemma A.1.13. Now, let h_0^{el} be the single-electron Hamiltonian of the decoupled system, i.e. with leads decoupled from the quantum system, and let ϖ_0 be a steady state with respect to h_0^{el}, i.e. ϖ_0 satisfies $\varpi_0(e^{it\mathrm{d}\Gamma(h_0^{el})} A e^{-it\mathrm{d}\Gamma(h_0^{el})}) = \varpi_0(A)$ for all $A \in \mathcal{A}_-(\mathfrak{h}^{el})$ and $t \in \mathbb{R}$. Then $[\rho_0^{el}, h_0^{el}] = 0$, and it has been proven by Aschbacher et al. [2] and Cornean et al. [26] that for any trace class operator $v_{el} \in \mathfrak{L}_1(\mathfrak{h}^{el})$

$$\varpi(\mathrm{d}\Gamma(v_{el})) = \lim_{t\to\infty} \varpi_t(\mathrm{d}\Gamma(v_{el})) = \mathrm{Tr}(\rho^{el} v_{el}) \tag{3.1}$$

with the density operator

$$\rho^{el} = W_-(h^{el}, h_0^{el}) \rho_0^{el} W_-(h^{el}, h_0^{el})^* + \sum_{\lambda \in \sigma_{pp}(h^{el})} E_{h^{el}}(\lambda) \rho_0 E_{h^{el}}(\lambda) \tag{3.2}$$

if $\sigma_{sc}(h^{el}) = \emptyset$. Recall that the wave operators are given by

$$W_-(h^{el}, h_0^{el}) = \operatorname*{s-lim}_{t\to\infty} e^{ith^{el}} e^{-ith_0^{el}} P^{ac}_{h_0^{el}},$$

cf. Appendix A.2. Obviously, ρ^{el} is a steady state with respect to h^{el}, i.e. it commutes with h^{el}, since the wave operators are intertwining. But even if ϖ_0 is an equilibrium state with respect to h_0^{el}, i.e. a function of h_0^{el}, ϖ is in general not an equilibrium state with respect to h^{el}. This is why we call ϖ respectively ρ^{el} a *non-equilibrium steady state*, in short NESS. It has the property that fluxes can be non-zero (non-equilibrium), but are constant over time (steady state), whereas in an equilibrium state all fluxes vanish. We use (3.1) to calculate the electric current of the many-electron system on the single-particle space. Let us stress again that this is only possible because we assumed that we can treat the electrons as non-interacting particles. This simplification implies that interaction effects like Coulomb blockade can not be handled directly in this framework.

Let us now define the current through the quantum system that is coupled to leads. In abstract mathematical terms, a *lead* is a subspace $\mathfrak{h}_l^{el}$ of the absolutely continuous subspace of h_0^{el} that reduces h_0^{el}. This is in contrast to the quantum system, whose spectrum is usually discrete. In particular, the orthogonal projection p_l^{el} onto $\mathfrak{h}_l^{el}$ commutes with h_0^{el}. To obtain the current into a lead $\mathfrak{h}_l^{el}$, we calculate the expectation value of the number of electrons entering this lead. The observable for the number of electrons is $\mathrm{d}\Gamma(p_l^{el})$. Its expectation value is in fact infinite. Nevertheless, the time derivative of $\mathrm{d}\Gamma(p_l^{el})$ in the steady state, given by the commutator

$$i[\mathrm{d}\Gamma(h^{el}), \mathrm{d}\Gamma(p_l^{el})] = i\mathrm{d}\Gamma([h^{el}, p_l^{el}]),$$

has a finite expectation value. This expectation value gives us the current $\mathfrak{J}_l$. A general definition of the current follows in Definition 3.1.1 in the next section. Assume for the moment that $v_{el} = h^{el} - h_0^{el} \in \mathfrak{L}_1(\mathfrak{h}^{el})$. Then $[h^{el}, p_l^{el}] = [v_{el}, p_l^{el}] \in \mathfrak{L}_1(\mathfrak{h}^{el})$ and, using the absolutely continuous part of the non-equilibrium steady state (3.2), we obtain for the current $\mathfrak{J}_l$ into the lead l

$$\mathfrak{J}_l = \varpi(i\mathrm{d}\Gamma([h^{el}, -p_l^{el}])) = i\,\mathrm{Tr}(W_-(h^{el}, h_0^{el})\rho_0^{el}W_-^*(h^{el}, h_0^{el})[v_{el}, -p_l^{el}]), \tag{3.3}$$

where the minus sign accounts for the negative charge of the electron. The pure point part of the NESS does not give any contribution to the current since

$$\mathrm{Tr}(E_{h^{el}}(\lambda)\rho_0^{el}E_{h^{el}}(\lambda)[h^{el}, p_l^{el}]) = \mathrm{Tr}(\rho_0 E_{h^{el}}(\lambda)[\lambda, -p_l^{el}]E_{h^{el}}(\lambda)) = 0$$

for any eigenvalue $\lambda \in \sigma_{pp}(h^{el})$. The Landauer-Büttiker formula for electrons states that

$$\begin{aligned}
\mathfrak{J}_l &= i\,\mathrm{Tr}(W_-(h^{el}, h_0^{el})\rho_0^{el}W_-^*(h^{el}, h_0^{el})[v_{el}, -p_l^{el}]) \\
&= 2\pi\int_{\mathbb{R}} \mathrm{d}\lambda \mathrm{Tr}\Big(\rho_0^{el}(\lambda)(t_{el}^*(\lambda)t_{el}(\lambda)p_l^{el}(\lambda) - t_{el}^*(\lambda)p_l^{el}(\lambda)t_{el}(\lambda)) \\
&\qquad\qquad + (2\pi i)^{-1}t_{el}(\lambda)[p_l^{el}(\lambda), \rho_0^{el}(\lambda)]\Big) \\
&= -\frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{d}\lambda\, \mathrm{Tr}\Big(\rho_0^{el}(\lambda)(s_{el}^*(\lambda)p_l^{el}(\lambda)s_{el}(\lambda) - p_l^{el}(\lambda))\Big).
\end{aligned} \tag{3.4}$$

Here, $s_{el}(\lambda)$ and $t_{el}(\lambda)$ are the scattering matrix respectively the transition matrix of the scattering system $\{h_0^{el}, h^{el}\}$, cf. Definition A.2.6. Furthermore, $\rho_0^{el}(\lambda)$ is the density matrix that we obtain from $(\Phi_{h_0^{el}}\rho_0^{el}f)(\lambda) = \rho_0^{el}(\lambda)(\Phi_{h_0^{el}}f)(\lambda)$ since $[h_0^{el}, \rho_0^{el}] = 0$, and

$p_l^{el}(\lambda)$ is defined similarly. The second equality follows directly from the first equality. Namely, using $s_{el} = 1 - 2\pi i\, t_{el}$ and the unitarity of s_{el} leads to

$$\begin{aligned}
&\rho_0^{el}(\lambda)(t_{el}^*(\lambda)t_{el}(\lambda)p_l^{el}(\lambda) - t_{el}^*(\lambda)p_l^{el}(\lambda)t_{el}(\lambda)) + (2\pi i)^{-1}t_{el}(\lambda)[p_l^{el}(\lambda), \rho_0^{el}(\lambda)] \\
&\quad = (2\pi i)^{-1}\rho_0^{el}(\lambda)(s_{el}^*(\lambda)t_{el}(\lambda)p_l^{el}(\lambda) - s_{el}^*(\lambda)p_l^{el}(\lambda)t_{el}(\lambda)) \\
&\quad = -(2\pi)^{-2}\rho_0^{el}(\lambda)(s_{el}^*(\lambda)p_l^{el}(\lambda)s_{el}(\lambda) - p_l^{el}(\lambda)).
\end{aligned}$$

This formula illustrates that the flux arises as a difference between the original observable and its image under the unitary transformation given by s^{el}. The formula (1.1) from the example in the introduction can be recovered from (3.4) if $\mathfrak{h}^{el} = \mathfrak{h}_l \oplus \mathfrak{h}_S \oplus \mathfrak{h}_r$ with left lead l, right lead r, and a discrete quantum system S. For the initial state

$$\rho_0^{el} = f_{FD}(h_l^{el} - \mu_l) \oplus \rho_S^{el} \oplus f_{FD}(h_r^{el} - \mu_r),$$

one can use $p_l^{el}(\lambda) + p_r^{el}(\lambda) = I_{\mathfrak{h}^{el}(\lambda)}$, $[p_j^{el}, \rho_0^{el}] = 0$, and $\big(t_{el}(\lambda)\big)_{jk} = p_j^{el}(\lambda)t_{el}(\lambda)p_k^{el}(\lambda)$ to obtain

$$\begin{aligned}
\mathfrak{J}_l &= -2\pi \int_{\mathbb{R}} \mathrm{d}\lambda \mathrm{Tr}\Big(\rho_r^{el}(\lambda)\big(t_{el}(\lambda)\big)_{lr}^*\big(t_{el}(\lambda)\big)_{lr}\Big) - \rho_l^{el}(\lambda)\big(t_{el}(\lambda)\big)_{rl}^*\big(t_{el}(\lambda)\big)_{rl}\Big) \\
&= -2\pi \int_{\mathbb{R}} \mathrm{d}\lambda (f_{FD}(\lambda - \mu_r) - f_{FD}(\lambda - \mu_l))\sigma_{lr}^{el}(\lambda),
\end{aligned}$$

where $\sigma_{lr}^{el}(\lambda) = \big|\big(t_{el}(\lambda)\big)_{lr}\big|^2$. Note that the initial state ρ_S^{el} of the quantum system does not have any influence on the resulting steady state current since the Hamiltonian h_S^{el} of the quantum system is pure point and this does not contribute to the current.

In the next chapter we prove an abstract Landauer-Büttiker formula for a general scattering system $\{H_0, H\}$ on $\mathfrak{H}$ for which the difference of some power of the resolvents is trace class. Also, we can calculate the flux of an arbitrary observable Q, not just for the electric current. For the case $V = H - H_0 \in \mathfrak{L}_1(\mathfrak{H})$, we can use the same concept as above to define the flux. We assume that H_0 and H are the decoupled and the coupled single-particle Hamiltonians of fermions that do not interact with eachother. Then the calculations on the Fock space $\mathfrak{F}_-(\mathfrak{H})$ reduce to a density operator ρ_0 on the single-particle space $\mathfrak{H}$ and the flux and the Landauer-Büttiker formula are

$$\begin{aligned}
\mathfrak{J}_l &= i\mathrm{Tr}(W_-(H, H_0)\rho_0 W_-(H, H_0)^*[V, Q]) \\
&= -\frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{d}\lambda\, \mathrm{Tr}\Big(\rho_0(\lambda)(Q(\lambda) - S^*(\lambda)Q(\lambda)S(\lambda))\Big).
\end{aligned} \tag{3.5}$$

Here, $S(\lambda)$ and $T(\lambda)$ are the scattering matrix and the transition matrix of the scattering system $\{H_0, H\}$ with respect to a spectral representation Φ of H_0. Furthermore, $Q(\lambda)$ and the density matrix $\rho_0(\lambda)$ are given by $\Phi Q \Phi^* = \mathcal{M}(Q(\lambda))$ and $\Phi\rho_0(\lambda)\Phi^* = \mathcal{M}(\rho_0(\lambda))$ since we assume that $[Q, H_0] = [\rho_0, H_0] = 0$.

For the general case in which we have only $(H - i)^{-N} - (H_0 - i)^{-N} \in \mathfrak{L}_1(\mathfrak{H})$ for some $N \in \mathbb{N}$, the flux in (3.5) is only a formal equation and we need to use a regularization in the definition of the flux to obtain a mathematically rigorous general Landauer-Büttiker formula. The rigorous definition of the flux of an observable, its assumptions, and the abstract Landauer-Büttiker formula are the subject of the next section.

3.1.2 A general Landauer-Büttiker formula

Let us first collect the assumptions on the scattering system $\{H_0, H\}$ and the initial state ρ_0. Recall that all Hamiltonians are assumed to be bounded from below. We assume

$$(H+\theta)^{-N} - (H_0+\theta)^{-N} \in \mathfrak{L}_1(\mathfrak{h}), \qquad \sigma_{sc}(H_0) = \sigma_{sc}(H) = \emptyset, \tag{A1}$$

for some $N \in \mathbb{N}$ and some $\theta > 0$. We already mentioned that the Landauer-Büttiker formalism is not limited to the electric current. We can calculate the flux of any observable $Q \in \mathfrak{L}(\mathfrak{h})$ that satisfies

$$Q^* = Q, \qquad [Q, H_0] = 0, \qquad Q(H+\theta)^{-N_Q},\ Q(H_0+\theta)^{-N_0} \in \mathfrak{B}(\mathfrak{h}), \tag{A2}$$

for some $N_Q, N_0 \in \mathbb{N}$ with $\theta > 0$ as in (A1). Important examples are $Q = P_l$, the number of electrons in lead l that we already mentioned in the introduction to this section, and $Q = H_l$, the energy of the electrons in lead l, if we assume that $H_0 = H_l \oplus H_S \oplus H_r$. The latter example gives us the energy flux into lead l. These two observables also allow us to calculate the entropy production rate, for which $\sum_{j\in\{l,r\}} \beta(H_j - \mu_j P_j)$ with inverse temperature β is the corresponding observable [2].

Let ρ_0 be the initial state of the system. To be able to handle unbounded observables, like H_l, and to get a flux observable that is trace class, we have stronger requirements on ρ_0 than mere boundedness. This is justified since in applications ρ_0 usually decays exponentially, e.g. like the Fermi-Dirac distribution $f_{FD}(\lambda) = (1+e^{\beta\lambda})^{-1}$. We assume for $N_{max} = \max\{2N_Q + N + 1, N_0\}$ that

$$\rho_0 = \rho_0^* \in \mathfrak{B}(\mathfrak{h}), \qquad [\rho_0, H_0] = 0, \qquad \rho_0(H_0+\theta)^{N_{max}} \in \mathfrak{B}(\mathfrak{h}), \tag{A3}$$

for $\theta > 0$ as in (A1). A density operator ρ_0 that derives from a quasi-free state always satisfies $0 \le \rho_0 \le 1$, cf. Appendix A.1. However, this is not relevant for the mathematical proofs, and we do not take it as a part of the assumptions. As already mentioned above, we obtain from [2, 26] that the steady state of the coupled system on the absolutely continuous part of H is given by

$$\rho = W_-(H, H_0)\rho_0 W_-^*(H, H_0).$$

Under this very general assumptions, the following definition gives a generalization of the current given by (3.5).

Definition 3.1.1. *Let H_0, H be densely defined, bounded from below self-adjoint operators on a separable Hilbert space $\mathfrak{h}$ which satisfy Assumption* (A1)*. Let $Q \in \mathfrak{L}(\mathfrak{h})$ satisfy Assumption* (A2) *and $\rho_0 \in \mathfrak{L}(\mathfrak{h})$ satisfy Assumption* (A3)*. Then the steady state* flux $\mathfrak{J}_{Q,\rho_0}$ *of Q in the steady state $\rho = |\mathrm{A}|\text{-}\lim_{t\to\infty} e^{-itH}\rho_0 e^{itH}$ is defined by*

$$\mathfrak{J}_{Q,\rho_0} = -\frac{i}{N}\mathrm{Tr}\Big(W_-(H,H_0)(H_0+\theta)^{2N_Q+N+1}\rho_0 W_-^*(H,H_0)(H+\theta)^{-N_Q} \times \big[(H+\theta)^{-N} - (H_0+\theta)^{-N}, Q\big](H+\theta)^{-N_Q}\Big).$$

The flux $\mathfrak{J}_{Q,\rho_0}$ is actually independent of the choice of θ. The definition formally

relates to (3.5) through the following relations. Note that

$$[(H+\theta)^{-N}, Q] = -\sum_{j=1}^{N}(H+\theta)^{-j}[H,Q](H+\theta)^{-(N+1-j)}.$$

Using this, the intertwining property $(H+\theta)^{-N}W_-(H,H_0) = W_-(H,H_0)(H_0+\theta)^{-N}$, $[H_0, Q] = 0$, and the cyclicity of the trace, we obtain formally

$$\begin{aligned}
&-\frac{i}{N}\mathrm{Tr}\Big(W_-(H,H_0)(H_0+\theta)^{2N_Q+N+1}\rho_0 W_-^*(H,H_0)(H+\theta)^{-N_Q} \\
&\qquad\qquad \times [(H+\theta)^{-N} - (H_0+\theta)^{-N}, Q](H+\theta)^{-N_Q}\Big) \\
&= -\frac{i}{N}\mathrm{Tr}\Big(W_-(H,H_0)(H_0+\theta)^{N+1}\rho_0 W_-^*(H,H_0)[(H+\theta)^{-N}, Q]\Big) \\
&= i\,\mathrm{Tr}\Big(W_-(H,H_0)\rho_0 W_-^*(H,H_0)[H,Q]\Big).
\end{aligned}$$

Compared to the definition of the steady state flux of [2], this definition has the advantage that the usage of the resolvents implies that we do not need a limiting process to obtain a regularization. The Landauer-Büttiker formula is the content of the following theorem.

Theorem 3.1.2. *Let H_0, H be densely defined, bounded from below self-adjoint operators on a separable Hilbert space $\mathfrak{h}$ which satisfy Assumption* (A1)*. Let $Q \in \mathfrak{L}(\mathfrak{h})$ satisfy Assumption* (A2) *and $\rho_0 \in \mathfrak{L}(\mathfrak{h})$ satisfy Assumption* (A3)*. Fix a spectral representation Φ_{H_0} of H_0^{ac}. Then*

$$\begin{aligned}
\mathfrak{J}_{Q,\rho_0} &= -2\pi\int_{\mathbb{R}}\mathrm{d}\lambda\mathrm{Tr}\Big(\rho_0(\lambda)(T^*(\lambda)T(\lambda)Q(\lambda) - T^*(\lambda)Q(\lambda)T(\lambda)) \\
&\qquad\qquad + (2\pi i)^{-1}T(\lambda)[Q(\lambda),\rho_0(\lambda)]\Big) \\
&= \frac{1}{2\pi}\int_{\mathbb{R}}\mathrm{d}\lambda\mathrm{Tr}\Big(\rho_0(\lambda)(S^*(\lambda)Q(\lambda)S(\lambda) - Q(\lambda))\Big),
\end{aligned}$$

where $S(\lambda)$, $T(\lambda)$, and $\rho_0(\lambda)$ are the scattering matrix, transition matrix, and density matrix, respectively, with respect to Φ_{H_0}, and $\Phi_{H_0}Q\Phi_{H_0}^* = \mathcal{M}(Q(\lambda))$.

We prefer to work with the representation of the flux in terms of $T(\lambda)$ since it is closer to the proof of the formula and at the same time closer to the heuristic picture of transition of particles through a system. Also, in applications we typically have $[Q,\rho_0] = 0$, whence this representation is usually as simple as the one in terms of the scattering matrix $S(\lambda)$.

The proof of Theorem 3.1.2 follows in Section 3.1.4. The idea is to first prove the formula for the case of $V = K - K_0 \in \mathfrak{L}_1(\mathfrak{H})$, then to reduce the general case to this situation. To prove the Landauer-Büttiker formula for $\{K_0, K\}$, we construct a special spectral representation from the trace class perturbation V in Section 3.1.3. We can derive formulae for the action of this representation on certain operator spectral integrals that arise in the stationary representation of the wave operators. Also, the stationary wave operators allow us to derive a very convenient formula for the transition matrix $T(\lambda)$ with respect to this spectral representation.

As mentioned earlier, Theorem 3.1.2 extends the result in [65], where the statement holds for $H - H_0 \in \mathfrak{L}_1(\mathfrak{h})$. A result similar to Theorem 3.1.2 was proven by Aschbacher et al. [2] for their version of the flux. In principle, their proof is similar to ours in the sense that they also use the stationary wave operators. However, it is rather abstract and relies on the existence of an abstract spectral representation that follows from results that can be found in [80]. In contrast, the special spectral representation we use gives us an explicit formula for the transition matrix. This makes the calculations in the proof very transparent and easier to follow. In Chapter 4 we even use a similar spectral representation to give a formula for the transition matrix that allows explicit numerical calculations. Furthermore, the tools that we develop for the proof can be used in the proof of the more general Landauer-Büttiker formula of Chapter 5.

The following corollary to Theorem 3.1.2 shows that all fluxes are zero if the initial state is an equilibrium state, i.e. a function of H_0. If the decoupled system H_0 decomposes into several subsystems, like the contacted quantum system of Section 3.1.1, we obtain an equilibrium state if we choose the same chemical potential in every subsystem, i.e. if the applied voltage is zero.

Corollary 3.1.3. *Let the assumptions of Theorem 3.1.2 be satisfied, and let one of the following hold.*

(i) ρ_0 *is an equilibrium sate, i.e.* $\rho_0 = \rho_0(H_0)$ *for some measurable* $\rho_0 : \mathbb{R} \to [0, \infty)$ *satisfying*

$$\sup_{\lambda \in \sigma(H_0)} \lambda^{N_{max}} \rho_0(\lambda) < \infty.$$

(ii) $Q = Q(H_0)$ *for some measurable* $Q : \mathbb{R} \to \mathbb{R}$ *satisfying*

$$\sup_{\lambda \in \sigma(H_0)} \lambda^{-N_0} |Q(\lambda)| < \infty.$$

Then all fluxes vanish, i.e. $\mathfrak{J}_{Q,\rho_0} = 0$.

Proof. Let (i) hold. Then we have $\rho_0(\lambda) \in \mathbb{R}$, whence

$$\mathfrak{J}_{Q,\rho_0} = \frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{d}\lambda \, \rho_0(\lambda) \mathrm{Tr}\big(S^*(\lambda) Q(\lambda) S(\lambda) - Q(\lambda)\big).$$

But $\mathrm{Tr}\big(S^*(\lambda)Q(\lambda)S(\lambda)\big) = \mathrm{Tr}\big(Q(\lambda)\big)$ by the cyclicity of the trace and the unitarity of $S(\lambda)$, whence the corollary follows.

If (ii) holds, the fact that $S(\lambda)$ is unitary and $Q(\lambda) \in \mathbb{R}$ commutes with $S(\lambda)$ gives us $S^*(\lambda)Q(\lambda)S(\lambda) = Q(\lambda)$, whence $\mathfrak{J}_{Q,\rho_0} = 0$. □

3.1.3 A formula for the transition matrix

For the remainder of this section, let $\{K_0, K\}$ be a scattering system where K_0 and K are bounded and $V = K - K_0 \in \mathfrak{L}_1(\mathfrak{H})$ is an additive trace class perturbation. In the following, we construct a special spectral representation of K_0^{ac} from this trace class perturbation, which was introduced by Behrndt et al. [12]. We use it in this section to derive a rather explicit formula for the transition matrix from the stationary

representation of the wave operators in terms of operator spectral integrals. It is also an important ingredient in the proof of Theorem 3.1.2, which follows in Section 3.1.4.

For arbitrary $C \in \mathfrak{L}_2(\mathfrak{H})$, we obtain from [9, Lemma I.3.11] that $CE_{K_0}(\cdot)C^*$, as a measure on $\mathcal{B}(\mathbb{R})$, is trace class-valued and of finite variation. It is absolutely continuous with respect to a Borel measure by [9, Prop. I.3.13], and thus the trace class-valued function $\lambda \mapsto CE_{K_0}((-\infty,\lambda))C^*$ is differentiable in the trace norm a.e. on $\mathbb{R}$ with derivative $Y(\lambda) \geq 0$. We define a measurable family of subspaces in $\mathfrak{H}$ by $\mathfrak{H}_\lambda = \mathrm{clo}\big(\mathrm{ran}(Y(\lambda))\big) \subset \mathfrak{H}$ with a family of orthogonal projections $P(\lambda)$, $\lambda \in \mathbb{R}$. Using this, we get an orthogonal projection $(Pf)(\lambda) = P(\lambda)f(\lambda)$ for all $f \in L^2(\mathbb{R}, \mathrm{d}\lambda, \mathfrak{H})$. The range of P is called the direct integral $L^2(\mathbb{R}, \mathrm{d}\lambda, \mathfrak{H}_\lambda) = \mathrm{ran}(P)$ of the family $\{\mathfrak{H}_\lambda\}_{\lambda\in\mathbb{R}}$. The next Lemma gives us a spectral representation of K_0^{ac}. It was proven by Behrndt et al. [12, Lemma A.1].

Lemma 3.1.4. *Take $L^2(\mathbb{R}, \mathrm{d}\lambda, \mathfrak{H}_\lambda)$ and $Y(\lambda)$ as above and assume $\mathfrak{H}_{K_0}^{ac} = \mathcal{K}(C)$, where*

$$\mathcal{K}(C) = \mathrm{clo}\Big(\mathrm{span}\big(E_{K_0}^{ac}(\Xi)\mathrm{ran}(C^*) \mid \Xi \in \mathcal{B}(\mathbb{R})\big)\Big). \tag{3.6}$$

Then the linear extension of the mapping Φ_{K_0} defined by

$$(\Phi_{K_0}E_{K_0}^{ac}(\Xi)C^*f)(\lambda) = \chi_\Xi(\lambda)\sqrt{Y(\lambda)}f, \qquad \lambda \in \mathbb{R}, \qquad f \in \mathfrak{H},$$

for $\Xi \in \mathcal{B}(\mathbb{R})$ onto the dense subspace $\mathrm{span}\big(E_{K_0}^{ac}(\Xi)\mathrm{ran}(C^*) \mid \Xi \in \mathcal{B}(\mathbb{R})\big)$ of $\mathfrak{H}_{K_0}^{ac}$ admits a unique continuation to an isometric isomorphism $\Phi_{K_0} : \mathfrak{H}_{K_0}^{ac} \to L^2(\mathbb{R}, \mathrm{d}\lambda, \mathfrak{H}_\lambda)$ such that

$$(\Phi_{K_0}E_{K_0}^{ac}(\Xi)g)(\lambda) = \chi_\Xi(\lambda)(\Phi_{K_0}g)(\lambda), \qquad g \in \mathfrak{H}_{K_0}^{ac},$$

holds for any $\Xi \in \mathcal{B}(\mathbb{R})$.

Define $C = \sqrt{|V|} \in \mathfrak{L}_2(\mathfrak{H})$ and $Z = \mathrm{sgn}(V) \in \mathfrak{B}(\mathfrak{H})$. Then C and Z are self-adjoint and $V = CZC$. If condition (3.6) is not satisfied, we still get a spectral representation. Observe that $\mathcal{K}(C)$ reduces K_0^{ac} since for $g \in \mathcal{K}(C)$ and partitions $\mathcal{J}_\epsilon^r$ of $[-r, r)$ with $r, \epsilon > 0$ such that $|\mathcal{J}_\epsilon^r| = \epsilon = r^{-1}$, there exist $\lambda_{\mathcal{J}_\epsilon^r,\Xi} \in \mathbb{R}$ such that

$$K_0^{ac}g = \lim_{r\to\infty} \sum_{\Xi\in\mathcal{J}_\epsilon^r} \lambda_{\mathcal{J}_\epsilon^r,\Xi} \underbrace{E_{K_0}^{ac}(\Xi)g}_{\in\mathcal{K}(C)} \in \mathcal{K}(C). \tag{3.7}$$

This implies that we may apply the construction of Lemma 3.1.4 to $K_0^{ac} \restriction \mathcal{K}(C)$ and thus obtain a spectral representation Φ_C. For any spectral representation $\Phi_C^\perp$ of $K_0^{ac} \restriction \mathcal{K}(C)^\perp$, we get a spectral representation $\Phi_{K_0} = \Phi_C \oplus \Phi_C^\perp$ of K_0^{ac}. For the remainder of this chapter, Φ_{K_0} denotes a spectral representation of K_0^{ac} that we obtain in this manner. For $f \in \mathfrak{H}_{K_0}^{ac}$ we write $\Phi_{K_0}f = \check{f}$, and for $A \in \mathfrak{L}(\mathfrak{H})$ commuting with K_0, we write $(\Phi_{K_0}Af)(\lambda) = \check{A}(\lambda)\check{f}(\lambda)$.

Since $V = K - K_0$ is trace class, the wave operators $W_\pm(K, K_0)$ exist and are complete by the Kato-Rosenblum theorem, cf. Appendix A.2. This implies that the scattering operator S is unitary. Note that the wave operators $W_\pm(K, K_0)$ have the following stationary representations. We have

$$\operatorname*{s-lim}_{\epsilon\to+0} W_{K,\pm}(\epsilon) = W_\pm(K, K_0),$$

where

$$W_{K,\pm}(\epsilon) = \int_{\mathbb{R}} (1 - (K - \lambda \pm i\epsilon)^{-1} V) \mathrm{d}E^{ac}_{K_0}(\lambda),$$

which is equivalent to

$$W_{K,\pm}(\epsilon) = \int_{\mathbb{R}} \mathrm{d}E_K(\lambda)(1 + V(K_0 - \lambda \mp i\epsilon)^{-1}) P^{ac}_{K_0}.$$

The following Lemma describes the action of the transformation Φ_{K_0} on operator spectral integrals of this kind. For a short introduction into operator spectral integrals, see Appendix A.2. Since we use this lemma also in Chapter 5, we give a more general formulation and do not use the fact that $C = C^*$ in our case.

Lemma 3.1.5. *Let $X : \mathbb{R} \to \mathfrak{B}(\mathfrak{H})$ be strongly continuous. If the operator spectral integral*

$$L = \int_{\mathbb{R}} \mathrm{d}E^{ac}_{K_0}(\lambda) C^* X(\lambda) \tag{3.8}$$

exists, then

$$(\Phi_{K_0} L f)(\lambda) = \sqrt{Y(\lambda)} X(\lambda) f, \qquad \lambda \in \mathbb{R}, \qquad f \in \mathfrak{H}, \tag{3.9}$$

holds. If in addition the operator spectral integral

$$L^* = \int_{\mathbb{R}} X^*(\lambda) C \mathrm{d}E^{ac}_{K_0}(\lambda)$$

exists, then

$$L^* \Phi^*_{K_0} \check{f} = \int_{\mathbb{R}} \mathrm{d}\lambda\, X^*(\lambda) \sqrt{Y(\lambda)} \check{f}(\lambda), \qquad f = \Phi^*_{K_0} \check{f} \in \mathfrak{H}^{ac}_{K_0}.$$

Proof. First, consider the interval $[-r, r)$ for some $r > 0$. Let $\mathcal{J}^r_\epsilon$, $\epsilon > 0$, be a family of partitions of $[-r, r)$ such that $|\mathcal{J}^r_\epsilon| = \epsilon$. Let further $\lambda^r_\epsilon : \mathcal{J}^r_\epsilon \to [-r, r)$ satisfy $\lambda^r_\epsilon(\Xi) \in \Xi$ for all $\Xi \in \mathcal{J}^r_\epsilon$. Then for

$$L_r f = \int_{-r}^{r} \mathrm{d}E^{ac}_{K_0}(\lambda) C^* X(\lambda) f, \qquad f \in \mathfrak{H},$$

by definition we have

$$L_r f = \lim_{\epsilon \to 0} \sum_{\Xi \in \mathcal{J}^r_\epsilon} E^{ac}_{K_0}(\Xi) C^* X(\lambda^r_\epsilon(\Xi)) f.$$

Since Φ_{K_0} is continuous and $\mathrm{ran}(L_r) \subset \mathcal{K}(C)$, we have

$$\begin{aligned}(\Phi_{K_0} L_r f)(\lambda) &= \lim_{\epsilon \to 0} \sum_{\Xi \in \mathcal{J}^r_\epsilon} (\Phi_{K_0} E^{ac}_{K_0}(\Xi) C^* X(\lambda^r_\epsilon(\Xi)) f)(\lambda) \\ &= \lim_{\epsilon \to 0} \sum_{\Xi \in \mathcal{J}^r_\epsilon} \chi_\Xi(\lambda) \sqrt{Y(\lambda)} X(\lambda^r_\epsilon(\Xi)) f\end{aligned}$$

for a.e. $\lambda \in [-r, r)$. Let $\Xi_\epsilon(\lambda)$ be the unique element in $\mathcal{J}^r_\epsilon$ that contains λ. Since X is

continuous, we obtain

$$(\Phi_{K_0} L_r f)(\lambda) = \lim_{\epsilon \to 0} \sqrt{Y(\lambda)} X(\lambda_\epsilon^r(\Xi_\epsilon(\lambda))) f = \sqrt{Y(\lambda)} X(\lambda) f.$$

Equation (3.9) follows if we let $r \to \infty$. The adjoint relation (3.1.5) follows easily from

$$\begin{aligned}\Big\langle g, \int_{\mathbb{R}} X^*(\lambda) C \mathrm{d}E_{K_0}^{ac}(\lambda) f \Big\rangle &= \Big\langle \int_{\mathbb{R}} \mathrm{d}E_{K_0}^{ac}(\lambda) C^* X(\lambda) g, f \Big\rangle \\ &= \int_{\mathbb{R}} \mathrm{d}\lambda \Big\langle \sqrt{Y(\lambda)} X(\lambda) g, (\Phi_{K_0} f)(\lambda) \Big\rangle \\ &= \Big\langle g, \int_{\mathbb{R}} \mathrm{d}\lambda \, X^*(\lambda) \sqrt{Y(\lambda)} (\Phi_{K_0} f)(\lambda) \Big\rangle\end{aligned}$$

for all $g \in \mathfrak{H}$. □

In the following Lemma we calculate the transition matrix $\check{T}(\lambda)$ of $\{K_0, K\}$ with respect to this spectral representation Φ_{K_0} of K_0^{ac}. Furthermore, in Corollary 3.1.7 we prove a relation between the perturbation V and the transition matrix that is an important ingredient in the proof of the Landauer-Büttiker formula in this chapter as well as in Chapter 5. Both lemmas use the relations of the previous Lemma 3.1.5.

Proposition 3.1.6. *For a.e. $\lambda \in \mathbb{R}$, the transition matrix satisfies*

$$\check{T}(\lambda) = \sqrt{Y(\lambda)} J(\lambda + i0) \sqrt{Y(\lambda)},$$

where

$$J(\lambda + i0) = \lim_{\epsilon \to +0} Z - ZC(K - \lambda - i\epsilon)^{-1} CZ$$

and the limit is taken in the Hilbert-Schmidt norm.

Proof. We have

$$\begin{aligned}-2\pi i \, T^* &= W_-^*(K, K_0) W_-(K, K_0) - W_-^*(K, K_0) W_+(K, K_0) \\ &= \operatorname*{s-lim}_{\delta \to +0} \operatorname*{w-lim}_{\epsilon \to +0} W_{K,-}^*(\epsilon) \big(W_{K,-}(\delta) - W_{K,+}(\delta) \big).\end{aligned}$$

Since we know that these limits exist, it suffices to calculate the pointwise limits. Hence, for $\check{f} \in L^2(\mathbb{R}, \mathrm{d}\lambda, \mathfrak{H}_\lambda)$ we consider

$$\begin{aligned}&\lim_{\epsilon \to +0} \Big(\Phi_{K_0} W_{K,-}^*(\epsilon) \big(W_{K,-}(\delta) - W_{K,+}(\delta) \big) \Phi_{K_0}^* \check{f} \Big)(\lambda) \\ &\quad = \lim_{\epsilon \to +0} \Big(\Phi_{K_0} \int_{\mathbb{R}} \mathrm{d}E_{K_0}^{ac}(\nu) \big(1 - V(K - \nu + i\epsilon)^{-1} \big) \int \mathrm{d}E_K(\mu) \\ &\qquad\qquad \times \big(1 + V(K_0 - \mu + i\delta)^{-1} - 1 - V(K_0 - \mu - i\delta)^{-1} \big) P_{K_0}^{ac} \Phi_{K_0}^* \check{f} \Big)(\lambda) \\ &\quad = \lim_{\epsilon \to +0} \Big(\Phi_{K_0} \int_{\mathbb{R}} \mathrm{d}E_{K_0}^{ac}(\nu) \big(1 - V(K - \nu + i\epsilon)^{-1} \big) V \\ &\qquad\qquad \times \big((K_0 - \nu + i\delta)^{-1} - (K_0 - \nu - i\delta)^{-1} \big) P_{K_0}^{ac} \Phi_{K_0}^* \check{f} \Big)(\lambda),\end{aligned}$$

where we used Lemma A.2.19. We get

$$\begin{aligned}
&\lim_{\epsilon\to+0}\Big(\Phi_{K_0}W_{K,-}^*(\epsilon)(W_{K,-}(\delta)-W_{K,+}(\delta))\Phi_{K_0}^*\check{f}\Big)(\lambda)\\
&\quad=\lim_{\epsilon\to+0}\Big(\Phi_{K_0}\int_{\mathbb{R}}\mathrm{d}E_{K_0}^{ac}(\nu)C\big(Z-ZC(K-\nu+i\epsilon)^{-1}CZ\big)\\
&\qquad\qquad\times\int_{\mathbb{R}}\big((\mu-\nu+i\delta)^{-1}-(\mu-\nu-i\delta)^{-1}\big)C\mathrm{d}E_{K_0}^{ac}(\mu)\Phi_{K_0}^*\check{f}\Big)(\lambda)\\
&\quad=-\lim_{\epsilon\to+0}2i\sqrt{Y(\lambda)}(Z-ZC(K-\lambda+i\epsilon)^{-1}CZ)\int_{\mathbb{R}}\frac{\delta}{(\mu-\lambda)^2+\delta^2}\sqrt{Y(\mu)}\mathrm{d}\mu\check{f}(\mu).
\end{aligned}$$

Since $C\in\mathfrak{L}_2(\mathfrak{H})$, the limit

$$ZC(K-\lambda\pm i0)^{-1}CZ=\lim_{\epsilon\to+0}ZC(K-\lambda\pm i\epsilon)^{-1}CZ$$

exists in the Hilbert-Schmidt norm by Lemma A.2.21. Furthermore, Lemma A.2.20 gives us

$$\int_{\mathbb{R}}\frac{\delta}{(\mu-\lambda)^2+\delta^2}\widehat{g}(\mu)\mathrm{d}\mu\ \stackrel{\delta\to0}{\longrightarrow}\ \pi\widehat{g}(\lambda).$$

Thus, taking the limits $\epsilon\to+0$ and $\delta\to+0$, we arrive at

$$-2\pi i\,T^*(\lambda)=-2\pi i\sqrt{Y(\lambda)}(Z-ZC(K-\lambda+i0)^{-1}CZ)\sqrt{Y(\lambda)},$$

which proves the Lemma. □

With the representation of $T(\lambda)$ of Proposition 3.1.6, it is easy to derive the following relation between T and $VW_-(K,K_0)$.

Corollary 3.1.7. *For a.e.* $\lambda\in\mathbb{R}$

$$T(\lambda)=(\Phi_{K_0}P_{K_0}^{ac}VW_-(K,K_0)\Phi_{K_0}^*)(\lambda,\lambda),\tag{3.10}$$

where

$$(\Phi_{K_0}P_{K_0}^{ac}VW_-(K,K_0)f)(\lambda)=\int_{\mathbb{R}}\mathrm{d}\mu(\Phi_{K_0}P_{K_0}^{ac}VW_-(K,K_0)\Phi_{K_0}^*)(\lambda,\mu)\check{f}(\mu)$$

for $f\in\mathfrak{H}_{K_0}^{ac}$.

Proof. $P_{K_0}^{ac}VW_-(K,K_0)$ is a trace class operator on $\mathfrak{H}_{K_0}^{ac}$. Hence, the spectral representation transforms it into an integral operator with kernel $(\Phi_{K_0}VW_-(K,K_0)\Phi_{K_0}^*)(\lambda,\mu)$ for a.e. $\lambda,\mu\in\mathbb{R}$. The diagonal $\mu=\lambda$ is well-defined for a.e. $\lambda\in\mathbb{R}$ (cf. [9, p. 401]). For $n\in\mathbb{N}$ choose $\Lambda_n\subset(-n,n)$ such that $|(-n,n)\setminus\Lambda_n|<n^{-1}$ and $C(K-\lambda-i\epsilon)^{-1}C$ converges uniformly for $\lambda\in\Lambda_n$. We can always find such a Λ_n by Egorov's theorem (cf. Lemma A.2.22). Observe that

$$P_{K_0}^{ac}VW_-(K,K_0)=\lim_{n\to\infty}P_{K_0}^{ac}VW_-(K,K_0)E_{K_0}(\Lambda_n)$$

in the trace norm. Thus,

$$\begin{aligned}
&(\Phi_{K_0} P^{ac}_{K_0} V W_-(K,K_0)\Phi^*_{K_0}\check{f})(\lambda)\\
&\quad= \lim_{n\to\infty}\lim_{\epsilon\to+0}\Big(\Phi_{K_0}P^{ac}_{K_0}\int_{\Lambda_n} V(1-(K-\mu-i\epsilon)^{-1}V)\mathrm{d}E^{ac}_{K_0}(\mu)\Phi^*_{K_0}\check{f}\Big)(\lambda)\\
&\quad= \lim_{n\to\infty}\lim_{\epsilon\to+0}\int_{\Lambda_n}\mathrm{d}\mu\,\sqrt{Y(\lambda)}(Z-ZC(K-\mu-i\epsilon)^{-1}CZ)\sqrt{Y(\mu)}\check{f}(\mu)
\end{aligned}$$

for all $\check{f}\in L^2(\mathbb{R},d\lambda,\mathfrak{H}_\lambda)$. But $C(K-\mu-i\epsilon)^{-1}C$ converges uniformly for $\mu\in\Lambda_n$ as $\epsilon\to+0$. This implies that we may take the limit inside the integral, whence the integral kernel is given by

$$(\Phi_{K_0}P^{ac}_{K_0}VW_-(K,K_0)\Phi^*_{K_0})(\lambda,\mu)=\sqrt{Y(\lambda)}(Z-ZC(K-\mu-i0)^{-1}CZ)\sqrt{Y(\mu)}$$

for a.e. $\lambda,\mu\in\mathbb{R}$. Thus, the Lemma follows from Proposition 3.1.6. □

3.1.4 Proof of Theorem 3.1.2

In this section we prove the Landauer-Büttiker formula of Theorem 3.1.2. We begin with the following proposition, which tells us that for $K-K_0\in\mathfrak{L}_1(\mathfrak{H})$, the flux for observables that live on the pure point part of K_0 is zero. This is implied by the Landauer-Büttiker formula. However, we have to prove it beforehand since we use it in the proof. The reason for this is the special spectral representation Φ_{K_0} of K_0^{ac}, as we will point out in the course of the proof of the Landauer-Büttiker formula.

Proposition 3.1.8. *Let $\{K_0,K\}$ be a scattering system such that K_0,K are bounded, $K-K_0\in\mathfrak{L}_1(\mathfrak{H})$, and $\sigma_{sc}(K)=\sigma_{sc}(K_0)=\emptyset$. Let $Q\in\mathfrak{B}(\mathfrak{H})$ with $[Q,K_0]=0$, and $\rho_0\in\mathfrak{B}(\mathfrak{H})$ with $[\rho_0,K_0]=0$. For $Q=Q_{pp}\oplus Q_{ac}$ with respect to $\mathfrak{H}=\mathfrak{H}^{pp}_{K_0}\oplus\mathfrak{H}^{ac}_{K_0}$, we have*

$$\mathrm{Tr}(W_-(K,K_0)\rho_0W_-^*(K,K_0)[V,Q_{pp}])=0.$$

The general idea of the proof is that the statement is obvious if Q_{pp} is a one-dimensional projection and the general case can be reduced to such a situation. We prove in Lemma 3.1.9 that we can approximate Q_{pp} with suitable pure point operators. Also, recall that $\sigma_{sc}(K_0^{ac})=\emptyset$ by assumption.

Lemma 3.1.9. *Let the assumptions of Proposition 3.1.8 hold. Then there is a sequence $\{Q^{pp}_m\}_{m\in\mathbb{N}}$ of bounded self-adjoint operators such that $\text{s-lim}_{m\to\infty}Q^{pp}_m=Q_{pp}$ and each operator Q^{pp}_m commutes with K_0^{pp} and is pure point.*

Proof. Since K_0^{pp} is pure point, we can choose a spectral representation $\Phi_{K_0^{pp}}$ such that

$$\Phi_{K_0^{pp}}K_0^{pp}\Phi^*_{K_0^{pp}}=\bigoplus_{\lambda\in\sigma_{pp}(K_0)}\lambda\, I_{\mathcal{H}(\lambda)},\qquad \Phi_{K_0^{pp}}\mathfrak{H}=\bigoplus_{\lambda\in\sigma_{pp}(K_0)}\mathcal{H}(\lambda). \tag{3.11}$$

Since Q_{pp} commutes with K_0^{pp}, there is a family $\{Q_{pp}(\lambda)\}_{\lambda\in\sigma_{pp}(K_0)}$ of bounded self-adjoint operators on $\mathcal{H}(\lambda)$ satisfying

$$\sup_{\lambda\in\sigma_{pp}(K_0)}\|Q_{pp}(\lambda)\|_{\mathcal{H}(\lambda)}=\|Q_{pp}\|_{\mathfrak{H}}$$

such that Q_{pp} is unitarily equivalent to $\bigoplus_{\lambda\in\sigma_{pp}(K_0)} Q_{pp}(\lambda)$.

The von Neumann theorem [55, Theorem X.2.1] tells us that for each self-adjoint operator $Q_{pp}(\lambda)$, $\lambda \in \sigma_{pp}(K_0)$, there is a sequence $\{C_m(\lambda)\}_{m\in\mathbb{N}}$ of self-adjoint Hilbert-Schmidt operators on $\mathcal{H}(\lambda)$ such that

$$\|C_m(\lambda)\|_{\mathfrak{L}_2(\mathcal{H}(\lambda))} \leq \frac{1}{m} \tag{3.12}$$

and $Q^{pp}_m(\lambda) = Q_{pp}(\lambda) + C_m(\lambda)$ is pure point. It follows that $\text{s-lim}_{m\to\infty} Q^{pp}_m(\lambda) = Q_{pp}(\lambda)$ for $\lambda \in \sigma_{pp}(K_0)$. Let the operator Q^{pp}_m be given by

$$Q^{pp}_m = \Phi^*_{K_0^{pp}}\Big(\bigoplus_{\lambda\in\sigma_{pp}(K_0)} Q^{pp}_m(\lambda)\Big)\Phi_{K_0^{pp}}.$$

Since $Q^{pp}_m(\lambda)$ is pure point for every $\lambda \in \sigma_{pp}(K_0)$, $m \in \mathbb{N}$, and we have estimate (3.12), Q^{pp}_m is bounded and pure point. From the decomposition (3.11) it is clear that Q^{pp}_m commutes with K^{pp}_0. Also, $Q_{pp} = \text{s-lim}_{m\to\infty} Q^{pp}_m$ by estimate (3.12). □

Proof of Proposition 3.1.8. We have to show that

$$\text{Tr}(W_-(K, K_0)\rho_0 W^*_-(K, K_0)[V, Q_{pp}]) = 0.$$

If the spectrum of Q_{pp} is pure point, K^{pp}_0 and Q_{pp} admit the representations

$$K^{pp}_0 = \sum_{n\in\mathbb{N}} \lambda^{(n)}_{K_0} P^{(n)}_{K_0^{pp}}, \qquad Q_{pp} = \sum_{l\in\mathbb{N}} \lambda^{(l)}_Q P^{(l)}_{Q_{pp}}$$

where $\lambda^{(n)}_{K_0}, \lambda^{(l)}_Q \in \mathbb{R}$ and $P^{(n)}_{K_0^{pp}}$, $P^{(l)}_{Q_{pp}}$ are eigenprojections of K^{pp}_0 and Q_{pp}, respectively. Since K^{pp}_0 and Q_{pp} commute, the eigenprojections $P^{(n)}_{K_0^{pp}}$ and $P^{(l)}_{Q_{pp}}$ commute as well. We set $P_{nl} = P^{(n)}_{K_0^{pp}} P^{(l)}_{Q_{pp}}$. Obviously, the P_{nl} are orthogonal projections. We obtain the representation

$$K^{pp}_0 = \sum_{n,l\in\mathbb{N}} \lambda^{(n)}_{K_0} Q_{nl}, \qquad Q_{pp} = \sum_{n,l\in\mathbb{N}} \lambda^{(l)}_Q Q_{nl},$$

where $\lambda^{(n)}_{K_0}, \lambda^{(l)}_Q \in \mathbb{R}$. Notice that $\sum_{n,l\in\mathbb{N}} Q_{nl} = P^{pp}_{K_0}$. Without loss of generality we can assume that the Q_{nl} are one dimensional orthogonal projections. Using this, the cyclicity of the trace, the intertwining property of the wave operators, and $[K_0, \rho_0] = 0$, we get that

$$\begin{aligned}
&\text{Tr}(W_-(K, K_0)\rho_0 W^*_-(K, K_0)[V, Q_{pp}]) \\
&= \sum_{n,l\in\mathbb{N}} \lambda^{(l)}_Q \text{Tr}(W_-(K, K_0)\rho_0 W^*_-(K, K_0)[K, Q_{nl}]) \\
&= \sum_{n,l\in\mathbb{N}} \lambda^{(l)}_Q \Big(\text{Tr}(W_-(K, K_0)\rho_0 K_0 W^*_-(K, K_0)Q_{nl}) \\
&\qquad\qquad - \text{Tr}(W_-(K, K_0)K_0\rho_0 W^*_-(K, K_0)Q_{nl})\Big) \\
&= 0.
\end{aligned}$$

If Q_{pp} is not pure point, then Lemma 3.1.9 gives us a sequence $\{Q_m^{pp}\}_{m\in\mathbb{N}}$ of bounded pure point self-adjoint operators acting on $\mathfrak{H}^{pp}$ such that $[K_0^{pp}, Q_m^{pp}] = 0$ for $m \in \mathbb{N}$ and s-$\lim_{m\to\infty} Q_m^{pp} = Q_{pp}$. Then

$$\begin{aligned}&\mathrm{Tr}(W_-(K,K_0)\rho_0 W_-^*(K,K_0)[V,Q_{pp}])\\ &\quad= \lim_{m\to\infty}\mathrm{Tr}(W_-(K,K_0)\rho_0 W_-^*(K,K_0)[V,Q_m^{pp}]).\end{aligned}$$

But Q_m^{pp} is pure point, whence by the above considerations

$$\mathrm{Tr}(W_-(K,K_0)\rho_0 W_-^*(K,K_0)[V,Q_{pp}]) = 0,$$

which proves Proposition 3.1.8. □

We use Proposition 3.1.8 in the proof of the next proposition, which provides a Landauer-Büttiker formula for bounded operators with an additive trace class perturbation. Later on, we reduce the general Landauer-Büttiker formula of Theorem 3.1.2 to this proposition. Thus, the following proposition is in fact the core of the proof of Theorem 3.1.2.

Proposition 3.1.10. *Let $\{K_0, K\}$ be a scattering system such that $K - K_0 \in \mathfrak{L}_1(\mathfrak{H})$ and $\sigma_{sc}(K) = \sigma_{sc}(K_0) = \emptyset$. Let $Q \in \mathfrak{B}(\mathfrak{H})$ with $[Q, K_0] = 0$ and $\varrho_0 \in \mathfrak{B}(\mathfrak{H})$ with $[\varrho_0, K_0] = 0$. Then*

$$\begin{aligned}\mathfrak{J}_{Q,K} &= i\,\mathrm{Tr}(W_-(K,K_0)\varrho_0 W_-^*(K,K_0)[V,Q])\\ &= -2\pi\int_{\mathbb{R}}\mathrm{d}\lambda\mathrm{Tr}\Big(\check{\varrho}_0(\lambda)(\check{T}^*(\lambda)\check{T}(\lambda)\check{Q}(\lambda) - \check{T}^*(\lambda)\check{Q}(\lambda)\check{T}(\lambda))\\ &\qquad\qquad + (2\pi i)^{-1}\check{T}(\lambda)[\check{Q}(\lambda),\check{\rho}_0(\lambda)]\Big).\end{aligned} \tag{3.13}$$

Proof. First note that Proposition 3.1.8 allows us to assume that

$$Q = Q \restriction \mathfrak{H}_{K_0}^{ac}. \tag{3.14}$$

Relation (3.14) is necessary since we work with spectral representations Φ_{K_0} of K_0^{ac}, not of the full Hamiltonian K_0, and in general $\Phi_{K_0}^*\Phi_{K_0} = P_{K_0}^{ac} \neq I_{\mathfrak{H}}$. During the proof we need to insert $\Phi_{K_0}^*\Phi_{K_0}$ to the left and right of Q, and (3.14) tells us that we are allowed to do this. We mention this again at the relevant point in the proof.

Let $W_{K,\pm}(\epsilon)$ be the stationary pre-wave operators for the wave operators $W_\pm(K, K_0)$. Recall the formulae

$$W_{K,\pm}(\epsilon) = \int_{\mathbb{R}}(1 - (H - \lambda \pm i\epsilon)^{-1}V)\mathrm{d}E_{H_0}^{ac}(\lambda)$$

and

$$W_{K,\pm}(\epsilon) = \int_{\mathbb{R}}\mathrm{d}E_H(\lambda)(1 + V(H_0 - \lambda \mp i\epsilon)^{-1})P_{K_0}^{ac}$$

for $V = CZC = K - K_0$, where $C = \sqrt{|V|}$ and $Z = \mathrm{sgn}(V)$. Also, $Y(\eta) = \frac{\mathrm{d}}{\mathrm{d}\eta}CE_{K_0}(\eta)C$

for a.e. $\eta \in \mathbb{R}$. Note that

$$\begin{aligned}&\lim_{\epsilon\to+0}\int_{\mathbb{R}} \mathrm{d}\eta\, \sqrt{Y(\eta)}\check{Q}(\eta)\sqrt{Y(\eta)}(\eta-\lambda\pm i\epsilon)^{-1}\\ &\quad= -\lim_{\epsilon\to+0}\int_{|\eta-\lambda|\geq\epsilon} \mathrm{d}\eta\sqrt{Y(\eta)}\check{Q}(\eta)\sqrt{Y(\eta)}(\lambda-\eta)^{-1} \mp i\pi\sqrt{Y(\lambda)}\check{Q}(\lambda)\sqrt{Y(\lambda)},\end{aligned} \tag{3.15}$$

in the Hilbert-Schmidt norm, cf. Lemma A.2.20. For $n \in \mathbb{N}$, use again Egorov's theorem, cf. Lemma A.2.22, to find a $\Lambda_n \subset (-n, n)$ satisfying $|(-n, n) \setminus \Lambda_n| < n^{-1}$ such that

$$C(H-\lambda\pm i\epsilon)C^{-1} \qquad \text{and} \qquad \int_{\mathbb{R}} \mathrm{d}\eta\, \sqrt{Y(\eta)}\check{Q}(\eta)\sqrt{Y(\eta)}(\eta-\lambda\pm i\epsilon)^{-1}$$

converge uniformly in the Hilbert-Schmidt norm for $\lambda \in \Lambda_n$ as $\epsilon \to +0$. Then

$$\operatorname*{s-lim}_{n\to\infty} E^{ac}_{K_0}(\Lambda_n) = P^{ac}_{K_0},$$

and we have

$$\mathfrak{J}_{Q,K} = \lim_{n\to\infty}\lim_{\epsilon\to+0}\lim_{\delta\to+0} -2\,\Im\mathrm{m}\big[\mathrm{Tr}\big(\varrho_0 E^{ac}_{K_0}(\Lambda_n)W^*_{K,-}(\epsilon)VQW_{K,-}(\delta)E^{ac}_{K_0}(\Lambda_n)\big)\big],$$

where ϱ_0 and Q commute with K_0 by the assumptions of the proposition. We used $\mathrm{Tr}(X_1X_3X_2) = \overline{\mathrm{Tr}(X_1X_2X_3)}$ for self-adjoint operators $X_j \in \mathfrak{B}(\mathfrak{H})$, $j = 1, 2, 3$, with $X_2 \in \mathfrak{L}_1(\mathfrak{H})$. We obtain

$$\begin{aligned}&E^{ac}_{K_0}(\Lambda_n)W^*_{K,-}(\epsilon)VQW_{K,-}(\delta)E^{ac}_{K_0}(\Lambda_n)\\ &\quad= E^{ac}_{K_0}(\Lambda_n)W^*_{K,-}(\epsilon)VQE^{ac}_{K_0}(\Lambda_n) - E^{ac}_{K_0}(\Lambda_n)W^*_{K,-}(\epsilon)VQ\widetilde{W}_{K,-}(\delta)E^{ac}_{K_0}(\Lambda_n),\end{aligned} \tag{3.16}$$

where

$$\widetilde{W}_{K,\pm}(\delta) = P^{ac}_{K_0} - W_{K,\pm}(\delta).$$

Let Φ_{K_0} be the spectral representation of K_0^{ac} that we obtain from $Y(\lambda) = \frac{\mathrm{d}}{\mathrm{d}\lambda}CE_{K_0}(\lambda)C$ using Lemma 3.1.4. Recall that for any $X \in \mathfrak{L}_1(\mathfrak{H})$, $\Phi_{K_0}X\Phi^*_{K_0}$ is an integral operator whose kernel has a well defined diagonal and

$$\mathrm{Tr}_{\mathfrak{H}}(X) = \int_{\mathbb{R}} \mathrm{d}\lambda \mathrm{Tr}_{\mathfrak{H}_\lambda}\big((\Phi_{K_0}X\Phi^*_{K_0})(\lambda,\lambda)\big).$$

Thus, using $[\varrho_0, K_0] = 0$, $[Q, K_0] = 0$, and Corollary 3.1.7, the first summand gives us

$$\begin{aligned}&\lim_{\epsilon\to+0}\mathrm{Tr}\big(\varrho_0 E^{ac}_{K_0}(\Lambda_n)W^*_{K,-}(\epsilon)VQE^{ac}_{K_0}(\Lambda_n)\big)\\ &\quad= \lim_{\epsilon\to+0}\int_{\Lambda_n} \mathrm{d}\lambda \mathrm{Tr}\big(\check{\varrho}_0(\lambda)(\Phi_{K_0}W^*_{K,-}(\epsilon)VP^{ac}_{K_0}\Phi^*_{K_0})(\lambda,\lambda)\check{Q}(\lambda)\big)\\ &\quad= \int_{\Lambda_n} \mathrm{d}\lambda \mathrm{Tr}\big(\check{\varrho}_0(\lambda)\check{T}^*(\lambda)\check{Q}(\lambda)\big).\end{aligned}$$

Since the wave operators $W_\pm(K, K_0)$ are complete, the scattering matrix $\check{S}(\lambda)$ is unitary.

Thus, the optical theorem from Lemma A.2.7 gives us

$$\Im\mathrm{m}[\check{T}^*(\lambda)] = (2i)^{-1}\big(\check{T}^*(\lambda) - \check{T}(\lambda)\big) = \pi\,\check{T}^*(\lambda)\check{T}(\lambda).$$

We use

$$\begin{aligned}&\mathrm{Tr}\big(\Im\mathrm{m}[\check{\varrho}_0(\lambda)\check{T}^*(\lambda)\check{Q}(\lambda)]\big)\\ &\quad= (2i)^{-1}\mathrm{Tr}\Big(\check{\varrho}_0(\lambda)\big(\check{T}^*(\lambda) - \check{T}(\lambda)\big)\check{Q}(\lambda) + \check{\varrho}_0(\lambda)\check{T}(\lambda)\check{Q}(\lambda) - \check{Q}(\lambda)\check{T}(\lambda)\check{\varrho}_0(\lambda)\Big)\end{aligned}$$

and the fact that $\|\check{T}(\lambda)\|_1$ is integrable and $\check{Q}(\lambda)$ and $\check{\varrho}_0(\lambda)$ are essentially bounded in $\lambda \in \mathbb{R}$ to obtain

$$\begin{aligned}&\lim_{n\to\infty}\lim_{\epsilon\to+0}\Im\mathrm{m}\big[\mathrm{Tr}\big(\varrho_0 E^{ac}_{K_0}(\Lambda_n)W^*_{K,-}(\epsilon)VQP^{ac}_{K_0}\big)\big]\\ &\quad= \pi\int_{\mathbb{R}}\mathrm{d}\lambda\mathrm{Tr}\big(\check{\varrho}_0(\lambda)\check{T}^*(\lambda)\check{T}(\lambda)\check{Q}(\lambda) + (2\pi i)^{-1}\check{T}(\lambda)[\check{Q}(\lambda),\check{\varrho}_0(\lambda)]\big).\end{aligned} \tag{3.17}$$

Let us now consider the second summand in (3.16). First note that we can use the resolvent equation to get

$$\begin{aligned}\widetilde{W}_{K,-}(\delta)E^{ac}_{K_0}(\Lambda_n) &= \int_{\Lambda_n}(K_0-\mu-i\delta)^{-1}\big(1-V(K-\mu-i\delta)^{-1}\big)V\mathrm{d}E^{ac}_{K_0}(\mu)\\ &= \int_{\Lambda_n}(K_0-\mu-i\delta)^{-1}CJ(\mu+i\delta)C\mathrm{d}E^{ac}_{K_0}(\mu),\end{aligned} \tag{3.18}$$

where we use the notation

$$J(\mu+i\epsilon) = Z - ZC(K-\mu-i\epsilon)^{-1}CZ.$$

Since

$$\begin{aligned}E^{ac}_0(\Lambda_n)W^*_{K,-}(\epsilon)V &= \int_{\Lambda_n}\mathrm{d}E^{ac}_{K_0}(\nu)\big(1-V(H-\nu+i\epsilon)^{-1}\big)V\\ &= \int_{\Lambda_n}\mathrm{d}E^{ac}_{K_0}(\nu)CJ(\nu-i\epsilon)C,\end{aligned}$$

the second summand in (3.16) leads to

$$\begin{aligned}&\Big(\Phi_{K_0}E^{ac}_{K_0}(\Lambda_n)W^*_{K,-}(\epsilon)VQ\widetilde{W}_{K,-}(\delta)E^{ac}_{K_0}(\Lambda_n)g\Big)(\lambda)\\ &\quad= \Big(\Phi_{K_0}\int_{\Lambda_n}\mathrm{d}E^{ac}_{K_0}(\nu)CJ(\nu-i\epsilon)C\int_{\mathbb{R}}\mathrm{d}E^{ac}_{K_0}(\eta)\Phi^*_{K_0}\Phi_{K_0}Q\Phi^*_{K_0}\\ &\qquad\times\Phi_{K_0}\int_{\Lambda_n}\mathrm{d}E^{ac}_{K_0}(\xi)\int_{\mathbb{R}}(\xi-\mu-i\delta)^{-1}CJ(\mu+i\delta)C\mathrm{d}E^{ac}_{K_0}(\mu)\Phi^*_{K_0}\check{g}\Big)(\lambda)\\ &\quad= \sqrt{Y(\lambda)}J(\lambda-i\epsilon)\int_{\mathbb{R}}\mathrm{d}\eta\sqrt{Y(\eta)}\check{Q}(\eta)\sqrt{Y(\eta)}\\ &\qquad\times\int_{\Lambda_n}\mathrm{d}\mu(\eta-\mu-i\delta)^{-1}J(\mu+i\delta)\sqrt{Y(\mu)}\check{g}(\mu)\end{aligned} \tag{3.19}$$

for $g \in \mathfrak{H}^{ac}_{K_0}$ and a.e. $\lambda \in \Lambda_n$. Here we used Lemma 3.1.5 to calculate the action of Φ_{K_0}. In the first equality of (3.19), we used that $Q = QP^{ac}_{K_0}$ allows us to insert $P^{ac}_{K_0} = \Phi^*_{K_0}\Phi_{K_0}$

to the left and to the right of Q. We proceed with the proof by calculating the trace of the imaginary part of (3.19). We obtain

$$\begin{aligned}
&\Im\mathrm{m}\Big[\mathrm{Tr}\Big(\varrho_0 E^{ac}_{K_0}(\Lambda_n) W^*_{K,-}(\epsilon) V Q \widetilde{W}_{K,-}(\delta) E^{ac}_{K_0}(\Lambda_n)\Big)\Big] \\
&\quad = (2i)^{-1} \int_{\Lambda_n} \mathrm{d}\lambda \mathrm{Tr}\Big(\check{\varrho}_0(\lambda) \sqrt{Y(\lambda)} J(\lambda - i\epsilon) \int_{\mathbb{R}} \mathrm{d}\eta \sqrt{Y(\eta)} \check{Q}(\eta) \\
&\qquad\qquad \times \sqrt{Y(\eta)} (\eta - \lambda - i\delta)^{-1} J(\lambda + i\delta) \sqrt{Y(\lambda)} \Big) \\
&\quad - (2i)^{-1} \int_{\Lambda_n} \mathrm{d}\lambda \mathrm{Tr}\Big(\check{\varrho}_0(\lambda) \sqrt{Y(\lambda)} J(\lambda - i\delta) \int_{\mathbb{R}} \mathrm{d}\eta \sqrt{Y(\eta)} \check{Q}(\eta) \\
&\qquad\qquad \times \sqrt{Y(\eta)} (\eta - \lambda + i\delta)^{-1} J(\lambda + i\epsilon) \sqrt{Y(\lambda)} \Big).
\end{aligned}$$

Using (3.15) and the fact that the individual factors inside the trace converge uniformly in $\lambda \in \Lambda_n$ gives us

$$\begin{aligned}
&\lim_{\epsilon \to +0} \lim_{\delta \to +0} \Im\mathrm{m}\Big[\mathrm{Tr}\Big(\varrho_0 E^{ac}_{K_0}(\Lambda_n) W^*_{K,-}(\epsilon) V Q \widetilde{W}_{K,-}(\epsilon) E^{ac}_{K_0}(\Lambda_n)\Big)\Big] \\
&\quad = \pi \int_{\Lambda_n} \mathrm{d}\lambda\, \mathrm{Tr}\Big(\check{\varrho}_0(\lambda) \sqrt{Y(\lambda)} J(\lambda - i0) \sqrt{Y(\lambda)} \check{Q}(\lambda) \sqrt{Y(\lambda)} J(\lambda + i0) \sqrt{Y(\lambda)} \Big) \\
&\quad = \pi \int_{\Lambda_n} \mathrm{d}\lambda\, \mathrm{Tr}(\check{\varrho}_0(\lambda) \check{T}^*(\lambda) \check{Q}(\lambda) \check{T}(\lambda)).
\end{aligned}$$

We can take the limit $n \to \infty$ to obtain

$$\begin{aligned}
&\Im\mathrm{m}\Big[\mathrm{Tr}\Big(\varrho_0 W^*_{K,-}(K, K_0) V Q (P^{ac}_{K_0} - W_{K,+}(K, K_0))\Big)\Big] \\
&\quad = \pi \int_{\mathbb{R}} \mathrm{d}\lambda\, \mathrm{Tr}(\check{\varrho}_0(\lambda) \check{T}^*(\lambda) \check{Q}(\lambda) \check{T}(\lambda)).
\end{aligned} \tag{3.20}$$

If we put together equations (3.17) and (3.20), we finally arrive at

$$\begin{aligned}
\mathfrak{J}_{Q,K} = -2\pi \int_{\mathbb{R}} \mathrm{d}\lambda \mathrm{Tr}\Big(\check{\varrho}_0(\lambda) (\check{T}^*(\lambda) \check{T}(\lambda) \check{Q}(\lambda) - \check{T}^*(\lambda) \check{Q}(\lambda) \check{T}(\lambda)) \\
+ (2\pi i)^{-1} \check{T}(\lambda) [\check{Q}(\lambda), \check{\varrho}_0(\lambda)] \Big).
\end{aligned}$$

□

To prove the general Landauer-Büttiker formula of Theorem 3.1.2, we reduce it to the situation of Proposition 3.1.10. To this end, we define

$$\varphi : \mathbb{R} \to \mathbb{R}, \qquad \varphi(x) = \begin{cases} -(x+\theta)^{-N} & \text{if } x \geq \inf\big(\sigma(H_0) \cup \sigma(H)\big), \\ 0 & \text{if } x < \inf\big(\sigma(H_0) \cup \sigma(H)\big), \end{cases} \tag{3.21}$$

for $\theta > -\inf\{\sigma(H_0) \cup \sigma(H)\}$. Since $(H+\theta)^{-N} - (H_0+\theta)^{-N} \in \mathfrak{L}_1(\mathfrak{h})$ by assumption, the wave operators $W_\pm(H, H_0)$ and

$$W_\pm(\varphi(H), \varphi(H_0)) = W_\pm\big(-(H+\theta)^{-N}, -(H_0+\theta)^{-N}\big)$$

exist and are complete for some $\theta > 0$. Now φ is continuously differentiable and φ' is strictly positive and locally of bounded variation. Hence, the invariance principle for wave operators applies and we obtain

$$W_\pm(H, H_0) = W_\pm\big(\varphi(H), \varphi(H_0)\big), \tag{3.22}$$

cf. Theorem A.2.12. Now, let $K_0 = \varphi(H_0)$, $K = \varphi(H)$, $\varrho_0 = (H_0 + \theta)^{N+1}\rho_0$, and $P^n_{K_0} = E_{H_0}\big((-\infty, n)\big)$. For $Q^n = QP^n_{K_0}$ we get that s-$\lim_{n\to\infty} Q^n = Q$, and

$$\begin{aligned}\mathfrak{J}_{Q,\rho_0} &= -\frac{i}{N}\mathrm{Tr}\Big(W_-(H, H_0)\rho_0(H_0 + \theta)^{2N_Q+N+1}W^*_-(H, H_0)\\ &\qquad \times (H + \theta)^{-N_Q}[(H + \theta)^{-N} - (H_0 + \theta)^{-N}, Q](H + \theta)^{-N_Q}\Big)\\ &= \lim_{n\to\infty}\frac{i}{N}\mathrm{Tr}\Big(W_-(K, K_0)\varrho_0 W^*_-(K, K_0)[K - K_0, Q^n]\Big).\end{aligned}$$

Hence, taking into account $\varrho_0 \in \mathfrak{B}(\mathfrak{H})$, and $Q^n \in \mathfrak{B}(\mathfrak{H})$, we can apply Theorem 3.1.10 to get

$$\mathfrak{J}_{Q,\rho_0} = \lim_{n\to\infty}\frac{1}{2\pi N}\int_{\mathbb{R}} \mathrm{d}\lambda\,\mathrm{Tr}\Big(\check{\varrho}_0(\lambda)(\check{S}^*(\lambda)\check{Q}^n(\lambda)\check{S}(\lambda) - \check{Q}^n(\lambda))\Big), \tag{3.23}$$

where

$$S = W^*_+(K, K_0)W_-(K, K_0) = W^*_+(H, H_0)W_-(H, H_0)$$

is the same for $\{K, K_0\}$ and $\{H, H_0\}$. Obviously, $\check{S}(\lambda)$ in equation (3.23) may be taken with respect to any spectral representation Φ_{K_0} of K^{ac}_0. Let Φ_{H_0} be a spectral representation of H^{ac}_0 on $L^2(\mathbb{R}, \mathrm{d}\lambda, \mathcal{H}_{H_0}(\lambda))$. Set

$$\varphi^{-1}(\lambda) = (-\lambda)^{-\frac{1}{N}} - \theta$$

such that $\varphi(\varphi^{-1}(\lambda)) = \lambda$. Define the unitary map Ψ_φ on $L^2(\mathbb{R}, \mathrm{d}\lambda, \mathcal{H}_{H_0}(\lambda))$ by

$$(\Psi_\varphi\check{f})(\mu) = \frac{1}{\sqrt{N}}(-\mu)^{-\frac{N+1}{2N}}\check{f}\big(\varphi^{-1}(\mu)\big), \tag{3.24}$$

which implies

$$(\Psi^*_\varphi\check{f})(\lambda) = \sqrt{N}\big(-\varphi(\lambda)\big)^{\frac{N+1}{2N}}\check{f}\big(\varphi(\lambda)\big).$$

Lemma 3.1.11. *Let Φ_{H_0} be any spectral representation of H^{ac}_0, and let Ψ_φ be given by (3.24). Then $\Psi_\varphi\Phi_{H_0}$ is a spectral representation of K^{ac}_0.*

Proof. Note that Ψ_φ maps $\mathcal{M}(A(\lambda))$ to $\mathcal{M}\big(A(\varphi^{-1}(\lambda))\big)$ for $A \in \mathfrak{L}(\mathfrak{H})$, $[A, K_0] = 0$. For a.e. $\lambda \in \mathbb{R}$, $g \in \mathfrak{H}$, and $\check{g} = \Psi_\varphi\Phi_{H_0}g$, we have

$$\big(\Psi_\varphi\Phi_{H_0}K_0\Phi^*_{H_0}\Psi^*_\varphi\check{g}\big)(\lambda) = \big(\Psi_\varphi\mathcal{M}(\varphi(\lambda))\check{g}\big)(\lambda) = \varphi\big(\varphi^{-1}(\lambda)\big)\check{g}(\lambda) = \lambda\,\check{g}(\lambda)$$

□

We may calculate $\mathfrak{J}_{Q,\rho_0}$ using this spectral representation $\Psi_\varphi\Phi_{H_0}$. Then

$$\begin{aligned}\big(\Psi_\varphi\Phi_{H_0}\varrho_0\Phi_{H_0}^*\Psi_\varphi^*\check{f}\big)(\lambda) &= \big(\Psi_\varphi\mathcal{M}\big((\lambda+\theta)^{N+1}\rho_0(\cdot)\big)\Psi_\varphi^*\check{f}\Big)(\lambda)\\ &= (-\lambda)^{-\frac{N+1}{N}}\rho_0\big(\varphi^{-1}(\lambda)\big)\check{f}(\lambda).\end{aligned}$$

Similarly,

$$\big(\Psi_\varphi\Phi_{H_0}T\Phi_{H_0}^*\Psi_\varphi^*\check{f}\big)(\lambda) = T(\varphi^{-1}(\lambda))\check{f}(\lambda)$$

and

$$\big(\Psi_\varphi\Phi_{H_0}Q\Phi_{H_0}^*\Psi_\varphi^*\check{f}\big)(\lambda) = Q(\varphi^{-1}(\lambda))\check{f}(\lambda).$$

We use $(\varphi^{-1})'(\lambda) = \frac{1}{N}(-\lambda)^{-\frac{N+1}{N}}$ to substitute $\mu = \varphi^{-1}(\lambda)$. Note that we also have $Q^n(\lambda) = \chi_{(-\infty,n)}(\lambda)Q(\lambda)$. We obtain

$$\begin{aligned}\mathfrak{J}_{Q,\rho_0} &= \lim_{n\to\infty}\frac{1}{2\pi N}\int_{\mathbb{R}}\mathrm{d}\lambda\,\mathrm{Tr}\Big((-\lambda)^{-\frac{N+1}{N}}\rho_0(\varphi^{-1}(\lambda))\\ &\qquad\qquad\times\Big(S^*(\varphi^{-1}(\lambda))Q^n(\varphi^{-1}(\lambda))S(\varphi^{-1}(\lambda)) - Q^n(\varphi^{-1}(\lambda))\Big)\Big)\\ &= \lim_{n\to\infty}\frac{1}{2\pi}\int_{-\infty}^{n}\mathrm{d}\mu\,\mathrm{Tr}\Big(\rho_0(\mu)\big(S^*(\lambda)Q(\lambda)S(\lambda) - Q(\lambda)\big)\Big)\\ &= 2\pi\int_{\mathbb{R}}\mathrm{d}\mu\,\mathrm{Tr}\Big(\rho_0(\mu)\big(T^*(\mu)Q(\mu)T(\mu) - T^*(\mu)T(\mu)Q(\mu)\big)\\ &\qquad\qquad+(2\pi i)^{-1}\,T(\lambda)[Q(\lambda),\rho_0(\lambda)]\Big).\end{aligned}$$

We can take the limit since $\|(\lambda+\theta)^{-N_0}Q(\lambda)\|$ and $\|(\lambda+\theta)^{N_0}\rho_0(\lambda)\|$ are essentially bounded in λ, and $\|T(\lambda)\|_1$ is integrable. Thus, Theorem 3.1.2 follows.

3.2 Application to a quantum LED toy model

As mentioned in the introduction to this chapter, we want to apply the Landauer-Büttiker formula of Theorem 3.1.2 to a model of a QD-LED based on the Jaynes-Cummings model of Section 2.3. The Jaynes-Cummings model describes an isolated quantum dot. To apply the Landauer-Büttiker formula, we have to introduce leads that couple to the Jaynes-Cummings model. These leads are modeled as semi-infinite one-dimensional lattices. Since the quantum dot is the optically active region, we restrict the electron-photon interaction to the quantum dot. Although there is no electron-photon interaction in the leads, it is important that the photons exist outside of the quantum dot. The quantum dot has pure point spectrum, but we can only measure fluxes on the absolutely continuous part. Thus, to be able to 'count' the photons, they have to exist in the leads. We stress that this is different to the common approach to view the quantum dot together with the photons as a black box that is contacted by purely electric leads.

Let us recall the basic ideas of the modeling of the QD-LED in the Landauer-Büttiker framework we presented in Section 1.2. The usual Landauer-Büttiker formalism for quasi-free electrons operates on the single-particle space. However, this does not mean that there is only a single electron. Since the electrons are non-interacting, the infinite

amount of electrons in the leads can be described by a density operator on the single-particle Hilbert space. This non-interaction condition implies that we can not take into account the Coulomb interaction. Since the Landauer-Büttiker formalism treats steady state currents, transient currents are also not covered by this approach.

In a QD-LED, the electron-photon interaction gives rise to an electron-electron interaction that is mediated by photons. To be able to work in the Landauer-Büttiker formalism, every electron has to interact with its own distinct copy of the electromagnetic field. This allows us to consider an electron together with its photon field as a 'single particle' in the sense of the Landauer-Büttiker formalism. Hence, we work with the single-particle Hilbert space $\mathfrak{h}^{el} \otimes \mathfrak{h}^{ph}$, where $\mathfrak{h}^{ph}$ is the Hilbert space of the photon field. This construction allows us to use the Landauer-Büttiker formalism developed in the previous section. Let us stress once more that we have infinitely many electrons and each electron has a photon field with an arbitrary number of photons, where the expectation value of the number of photons is finite for each single electron. We model this through a density operator on the single-particle Hilbert space $\mathfrak{h}^{el} \otimes \mathfrak{h}^{ph}$. Recall that this corresponds to the electrons being labled by the number of photons in their photon field. We mention again that a useful picture is that of every electron carrying a backpack filled with a certain amount of photons.

3.2.1 The mathematical model

Recall the generalized Jaynes-Cummings model from Section 2.3.3. The Hamiltonian is

$$H_S = h_S^{el} \otimes I_{ph} + I_{\mathfrak{h}_S^{el}} \otimes h^{ph} + \tau_{int} V_{int}, \qquad V_{int} = b^* \otimes a + b \otimes a^*,$$

with domain

$$\mathrm{dom}(H_S) = \mathrm{dom}(I_{\mathfrak{h}_S^{el}} \otimes h^{ph}) \subset \mathfrak{H}_S = \mathbb{C}^d \otimes \ell^2(\mathbb{N}_0)$$

for some $d \geq 2$. Here, the electron Hamiltonian h_S^{el} of the quantum dot acting on $\mathfrak{h}_S^{el} = \mathbb{C}^d$ has eigenvectors $\{e_0, e_1, \dots e_{d-1}\}$ corresponding to eigenvalues $\lambda_m = v_0 + m\omega_0$, where $v_0 \in \mathbb{R}$ is the ground state energy, and b^* and b are the ladder operators raising respectively lowering the energy level of the electron. Without loss of generality we assume $v_0 = 0$. Furthermore,

$$h^{ph} = \omega\, a^* a, \qquad h^{ph} \Upsilon_n = n\omega,$$

where a^* and a are the creation and annihilation operators on $\mathfrak{h}^{ph} = \mathfrak{F}_+(\mathbb{C}) = \ell^2(\mathbb{N}_0)$ and $\{\Upsilon_n\}_{n \in \mathbb{N}_0}$ is the canonical basis of $\ell^2(\mathbb{N}_0)$. This immediately implies

$$\sigma(h^{ph}) = \sigma_{pp}(h^{ph}) = \{n\omega \,|\, n \in \mathbb{N}_0\}.$$

We can interpret the electron space $\mathbb{C}^d$ as d adjacent sites of a one-dimensional lattice, and in this sense we model the electrons in the leads as free electrons living on a discrete semi-infinite lattice. Thus, the Hilbert spaces of the leads are $\mathfrak{h}_j^{el} = \ell^2(\mathbb{N})$, $j \in \{l, r\}$. The electron Hamiltonians of the leads are $h_j^{el} = -\Delta^D + v_j$ with a constant potential

bias $v_j \in \mathbb{R}$, $j \in \{l, r\}$. Here, Δ^D denotes the discrete Laplacian on $\ell^2(\mathbb{N})$ given by

$$(\Delta^D f)(1) = f(2) - 2f(1), \qquad (\Delta^D f)(x) = f(x+1) - 2f(x) + f(x-1), \qquad x \geq 2.$$

Note that the definition of $(\Delta^D f)(1)$ corresponds to $f(0) = 0$, i.e. to homogeneous Dirichlet boundary conditions. Obviously, Δ^D is a bounded self-adjoint operator. The photons in the leads are free, whence the total Hamiltonians of the leads are

$$H_j = h_j^{el} \otimes I_{ph} + I_{\mathfrak{h}_j^{el}} \otimes h^{ph}, \qquad j \in \{l, r\}.$$

To apply the Landauer-Büttiker formula, we need a scattering system $\{H_0, H\}$. In principle, we could use $H_l \oplus H_S \oplus H_r$ as unperturbed Hamiltonian. However, we want to analyze the contributions of the coupling of the leads and the electron-photon interaction to the resulting flux separately. Also, we want to be able to compare the system to the purely electric case. This is why we define the decoupled Hamiltonian H_0 with decoupled leads and without electron-photon interaction by

$$H_0 = h_0^{el} \otimes I_{ph} + I_{el} \otimes h^{ph}, \quad \operatorname{dom}(H_0) = \operatorname{dom}(I_{el} \otimes a^* a) \subset \mathfrak{H} = (\mathfrak{h}_l^{el} \oplus \mathfrak{h}_S^{el} \oplus \mathfrak{h}_r^{el}) \otimes \mathfrak{h}^{ph},$$

where $h_0^{el} = h_l^{el} \oplus h_S^{el} \oplus h_r^{el}$ is the decoupled electron Hamiltonian, which is bounded and self-adjoint. Since h^{ph} is also self-adjoint and bounded from below, H_0 is also self-adjoint and bounded from below. It remains to specify the coupling of the leads to the quantum dot. The physical idea behind the coupling is that the quantum dot has a left side and a right side and that the electrons may hop from the endpoints of the left and right lead into the left respectively right side of the dot. Hence, choose a basis $\{x_S^n\}_{n=0}^{d-1}$ of $\mathfrak{h}_S^{el}$. We consider $\{x_S^n\}_{n=0}^{d-1}$ as d sites of a one-dimensional finite lattice, where x_S^0 is the left side of the quantum dot and x_S^{d-1} is the right side of the quantum dot, cf. Figure 3.1. Furthermore, let $\{x_j^n\}_{n \in \mathbb{N}}$ be the canonical basis of $\mathfrak{h}_j^{el} = \ell^2(\mathbb{N})$, $j \in \{l, r\}$, which we consider to be the lattice sites of the leads. The coupling of the leads is given by

$$v_{el} = \begin{pmatrix} 0 & \langle x_S^0, \cdot \rangle x_l^1 & 0 \\ \langle x_l^1, \cdot \rangle x_S^0 & 0 & \langle x_r^1, \cdot \rangle x_S^{d-1} \\ 0 & \langle x_S^{d-1}, \cdot \rangle x_r^1 & 0 \end{pmatrix}.$$

It is obviously bounded and self-adjoint. We define the coupled electron Hamiltonian $h^{el} = h_0^{el} + \tau_{el} v_{el}$ for some coupling constant $\tau_{el} > 0$. Let $V_{el} = v_{el} \otimes I_{ph}$. We obtain the total Hamiltonian

$$H = H_0 + \tau_{el} V_{el} + \tau_{int} V_{int} = (H_l \oplus H_S \oplus H_r) + \tau_{el} V_{el}.$$

It models the quantum dot as a Jaynes-Cummings system contacted by two leads with free electrons subject to different constant potentials. Figure 3.1 shows a sketch of the system, using the well-known fact that the spectrum of the discrete Laplacian is $[0, 4]$, cf. Lemma 3.2.2. Note that H_S is self-adjoint and bounded from below by Lemma 2.3.1. It follows that H is self-adjoint and bounded from below since H_l, H_r, and V_{el} are also self-adjoint and bounded from below.

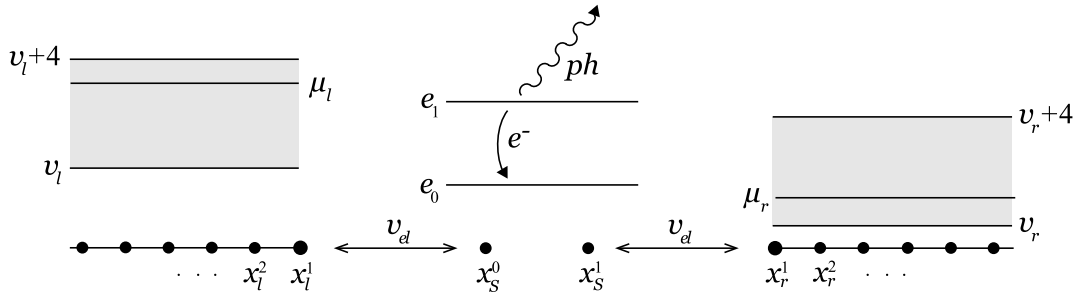

Figure 3.1: Jaynes-Cummings QD-LED with two energy levels

Since there is no electron-photon interaction in the leads, one might consider to work with the Hilbert spaces $\mathfrak{h}_j^{el}$, $j \in \{l, r\}$, and forget about the photons in the leads. We did already mention that this does not work since the quantum dot system is pure point, whence $\mathfrak{H}_S \cap \mathfrak{H}_{H_0}^{ac} = 0$. But then the photons do not exist in the absolutely continuous subspace of H_0, and the flux of the observable $I_{el} \otimes a^*a$ of the number of photons is always zero.

To obtain the Landauer-Büttiker formula from Theorem 3.1.2, we have to show that all assumptions of the theorem are satisfied. First note that since H_0 and H are densely defined, self-adjoint, and bounded from below, they are valid as Hamiltonians in the model. Concerning the Hamiltonians, it remains to check Assumption (A1), i.e. the trace class condition and the absence of singular continuous spectrum for H_0 and H.

We start with the trace class condition. Since $\mathrm{dom}(H) = \mathrm{dom}(H_0)$, we may define the symmetric, non-self-adjoint operator $V = V_{el} + V_{int}$ on $\mathrm{dom}(H_0)$.

Proposition 3.2.1. *We have $(H+\theta)^{-1} - (H_0+\theta)^{-1} \in \mathfrak{L}_1(\mathfrak{H})$ for $\theta > 0$ sufficiently large.*

Proof. First note that $(H_0+\theta)^{-1}$ and $(H+\theta)^{-1}$ are bounded for $\theta > 0$ sufficiently large since H_0 and H are bounded from below. We have

$$\begin{aligned}
&(H+\theta)^{-1} - (H_0+\theta)^{-1} \\
&\quad = (H_0+\theta)^{-1} V (H+\theta)^{-1} \\
&\quad = (H_0+\theta)^{-1} V (H_0+\theta)^{-1} - (H_0+\theta)^{-1} V (H_0+\theta)^{-1} V (H+\theta)^{-1}.
\end{aligned}$$

Since $\mathrm{dom}(H) = \mathrm{dom}(H_0)$ implies that $V(H+\theta)^{-1}$ is bounded, it suffices to show that $(H_0+\theta)^{-1} V (H_0+\theta)^{-1} \in \mathfrak{L}_1(\mathfrak{H})$. Using the spectral decomposition of h^{ph} with respect to $\mathfrak{h}^{ph} = \bigoplus_{n\in\mathbb{N}_0} \mathfrak{h}_n^{ph}$, where $\mathfrak{h}_n^{ph} = \mathbb{C}\Upsilon_n$, we obtain

$$(H_0+\theta)^{-1} = \bigoplus_{n\in\mathbb{N}_0} (h_0^{el} + n\omega + \theta)^{-1} \otimes I_{\mathfrak{h}_n^{ph}}. \tag{3.25}$$

We have

$$(H_0+\theta)^{-1} V (H_0+\theta)^{-1} = (H_0+\theta)^{-1} (V_{el} + V_{int}) (H_0+\theta)^{-1}.$$

But v_{el} is a finite rank operator and hence $\|v_{el}\|_1 < \infty$. Furthermore, $\mathfrak{h}_n^{ph}$ is obviously

one-dimensional for any $n \in \mathbb{N}$, and hence $\|I_{\mathfrak{h}_n^{ph}}\|_1 = 1$. From (3.25) and the fact that $V_{el} = v_{el} \otimes I_{ph}$, we obtain

$$\begin{aligned}\|(H_0+\theta)^{-1}V_{el}(H_0+\theta)^{-1}\|_1 &= \sum_{n\in\mathbb{N}_0} \|(h_0^{el}+n\omega+\theta)^{-1}v_{el}(h_0^{el}+n\omega+\theta)^{-1}\|_1 \\ &\leq \sum_{n\in\mathbb{N}_0} \|(h_0^{el}+n\omega+\theta)^{-2}\|\,\|v_{el}\|_1.\end{aligned}$$

Since h_0^{el} is bounded, we obtain

$$\|(h_0^{el}+n\omega+\theta)^{-1}\| = \sup_{\lambda\in\sigma(h_0^{el})} (\lambda+n\omega+\theta)^{-1} \leq \frac{\widetilde{\alpha}}{n+1} \tag{3.26}$$

for some $\widetilde{\alpha} > 0$, which immediately implies $\|(H_0+\theta)^{-1}V_{el}(H_0+\theta)^{-1}\|_1 < \infty$. For $n \in \mathbb{N}_0$ let p_n^{ph} be the orthogonal projection of $\mathfrak{h}^{ph}$ onto $\mathfrak{h}_n^{ph}$. We have

$$\begin{aligned}&(H_0+\theta)^{-1}\big(b^*\otimes a\big)(H_0+\theta)^{-1} \\ &\quad= \sum_{m,n\in\mathbb{N}_0} \big((h_0^{el}+m\omega+\theta)^{-1}b^*(h_0^{el}+n\omega+\theta)^{-1}\big)\otimes p_m^{ph}ap_n^{ph} \\ &\quad= \sum_{n\in\mathbb{N}} \big((h_0^{el}+(n-1)\omega+\theta)^{-1}b^*(h_0^{el}+n\omega+\theta)^{-1}\big)\otimes\big(\sqrt{n}\Upsilon_n\langle\Upsilon_n,\cdot\rangle\big).\end{aligned}$$

Since b^* has at most rank d and $\Upsilon_n\langle\Upsilon_n,\cdot\rangle$ has rank one, it holds that $\|b^*\otimes\Upsilon_n\langle\Upsilon_n,\cdot\rangle\|_1 \leq \widetilde{\gamma}$ for some $\widetilde{\gamma} > 0$. From relation (3.26) we get

$$\|(H_0+\theta)^{-1}\big(b^*\otimes a\big)(H_0+\theta)^{-1}\|_1 \leq \sum_{n\in\mathbb{N}} \frac{\widetilde{\gamma}\,\widetilde{\alpha}^2\sqrt{n}}{n(n+1)} < \infty.$$

Finally, $\|(H_0+\theta)^{-1}\big(b\otimes a^*\big)(H_0+\theta)^{-1}\|_1 = \|(H_0+\theta)^{-1}\big(b^*\otimes a\big)(H_0+\theta)^{-1}\|_1$ implies that $(H_0+\theta)^{-1}V(H_0+\theta)^{-1} \in \mathfrak{L}_1(\mathfrak{H})$. □

It remains to check the absence of the singular continuous spectrum. To show this we first obtain detailed information on the spectral properties of h_j^{el}, $j \in \{l,r\}$, and thus of H_0. We then use this to show that H does not have singular continuous spectrum. Recall that the discrete Laplacian on $\ell^2(\mathbb{N})$ with Dirichlet boundary condition is given by

$$(\Delta^D f)(1) = f(2) - 2f(1), \qquad (\Delta^D f)(x) = f(x+1) - 2f(x) + f(x-1), \qquad x \geq 2,$$

for $f \in \ell^2(\mathbb{N})$, and that $h_j^{el} = -\Delta^D + v_j$, $j \in \{l,r\}$, on $\mathfrak{h}_l = \mathfrak{h}_r = \ell^2(\mathbb{N})$. The following lemma about the eigenfunctions of the discrete Laplacian is well-known. For the convenience of the reader, we give a proof.

Lemma 3.2.2. *Let $j \in \{l,r\}$. We have $\sigma(h_j^{el}) = \sigma_{ac}(h_j^{el}) = [v_j, 4+v_j]$, and for $x \in \mathbb{N}$, $\lambda \in (v_j, 4+v_j)$, the normalized generalized eigenfunctions of h_j^{el} are given by*

$$g_j(x,\lambda) = \pi^{-\frac{1}{2}}(1-(-\lambda+2+v_j)^2/4)^{-\frac{1}{4}}\sin\big(\arccos((-\lambda+2+v_j)/2)x\big).$$

Proof. Let $j \in \{l, r\}$. We prove absolute continuity of the spectrum by showing that a complete set of generalized eigenfunctions is given by $\{g_j(x,\lambda) \,|\, \lambda \in (-2,2)\}$. Note that it suffices to calculate the spectrum of the operator $\Delta^D + 2$ given by

$$((\Delta^D + 2)f)(x) = f(x+1) + f(x-1), \qquad f \in \ell^2(\mathbb{N}), \qquad f(0) = 0.$$

The lemma then follows by replacing λ with $-\lambda + 2 + v_j$. Let $\lambda \in (-2,2)$ and

$$g_{\Delta^D}(x,\lambda) = \pi^{-\frac{1}{2}}(1-\lambda^2/4)^{-\frac{1}{4}} \sin\big(\arccos(\lambda/2)x\big)$$

Note that $g_{\Delta^D}(0,\lambda) = 0$, whence the boundary condition is satisfied. We substitute $\mu = \arccos(\lambda/2) \in (0,\pi)$, i.e. $\lambda = 2\cos(\mu)$, and obtain

$$\sin(\mu(x+1)) + \sin(\mu(x-1)) = 2\sin(\mu x)\cos(\mu),$$

whence $g_{\Delta^D}(x,\lambda)$ satisfies the eigenvalue equation. It is obvious that $g_{\Delta^D}(\cdot,\lambda) \notin \ell^2(\mathbb{N})$ for $\lambda \in (-2,2)$. To complete the proof of the lemma, it remains to prove the orthonormality and the completeness. For the orthonormality, we have to show that

$$\sum_{x\in\mathbb{N}} g_{\Delta^D}(x,\lambda) g_{\Delta^D}(x,\nu) = \delta(\lambda - \nu).$$

Let $\psi \in C_0^\infty((-2,2))$. We substitute $\mu = \arccos(\nu/2)$ and use $(1-y^2)^{\frac{1}{2}} = \sin(\arccos(y))$ to obtain

$$\begin{aligned}
&\int_{-2}^{2} \mathrm{d}\nu \sum_{x\in\mathbb{N}} g_{\Delta^D}(x,\lambda) g_{\Delta^D}(x,\nu)\psi(\nu) \\
&\quad = 2\pi^{-1} \int_0^\pi \mathrm{d}\mu \sum_{x\in\mathbb{N}} \frac{\sin(\mu)\sin\big(\arccos(\lambda/2)x\big)\sin(\mu x)}{(\sin(\mu))^{\frac{1}{2}}(\sin(\arccos(\lambda/2)))^{\frac{1}{2}}}\psi(2\cos(\mu)) \\
&\quad = (2\pi)^{-1} \int_0^\pi \mathrm{d}\mu \sum_{x\in\mathbb{N}} \frac{(\sin(\mu))^{\frac{1}{2}}}{(\sin(\arccos(\lambda/2)))^{\frac{1}{2}}}\Big(e^{i(\arccos(\lambda/2)-\mu)x} + e^{-i(\arccos(\lambda/2)-\mu)x} \\
&\qquad\qquad - e^{i(\arccos(\lambda/2)+\mu)x} - e^{-i(\arccos(\lambda/2)+\mu)x}\Big)\psi(2\cos(\mu)).
\end{aligned}$$

Observe that the Dirichlet kernel $\sum_{x\in\mathbb{N}_0}(e^{ixy} + e^{-ixy}) - 1 = 2\pi\,\delta(y)$ gives us

$$\begin{aligned}
&\int_{-2}^{2} \mathrm{d}\nu \sum_{x\in\mathbb{N}} g_{\Delta^D}(x,\lambda) g_{\Delta^D}(x,\nu)\psi(\nu) \\
&\quad = \int_0^\pi \mathrm{d}\mu \frac{(\sin(\mu))^{\frac{1}{2}}}{(\sin(\arccos(\lambda/2)))^{\frac{1}{2}}}\Big(\delta(\arccos(\lambda/2)-\mu) + \delta(\arccos(\lambda/2)+\mu)\Big)\psi(2\cos(\mu)).
\end{aligned}$$

Note that both $\arccos(\lambda/2) > 0$ and $\mu > 0$, whence $\delta(\arccos(\lambda/2)+\mu)$ is zero and

$$\int_{-2}^{2} \mathrm{d}\nu \sum_{x\in\mathbb{N}} g_{\Delta^D}(x,\lambda) g_{\Delta^D}(x,\nu)\psi(\nu) = \psi(\lambda).$$

Thus, the generalized eigenfunctions are orthonormal. Finally, using once more the substitution $\mu = \arccos(\nu/2)$, we get

$$\begin{aligned}
&\int_{-2}^{2} \mathrm{d}\nu \, g_{\Delta^D}(x,\nu) g_{\Delta^D}(y,\nu) \\
&\quad = \int_{-2}^{2} \mathrm{d}\nu \, (1-(\nu/2)^2)^{-\frac{1}{2}} \sin\big(\arccos(\nu/2)x\big) \sin\big(\arccos(\nu/2)y\big) \\
&\quad = 2\pi^{-1} \int_0^{\pi} \mathrm{d}\mu \, (\sin(\mu))^{-1} \sin(\mu) sin(\mu x) \sin(\mu y) \\
&\quad = \delta_{xy}
\end{aligned}$$

for $x, y \in \mathbb{N}$, whence the family of generalized eigenfunctions is also complete. □

We already noted that h^{ph} is pure point with $\sigma(h^{ph}) = \sigma_{pp}(h^{ph}) = \{n\omega \,|\, n \in \mathbb{N}_0\}$. The following corollary gives us the spectral properties of H_0.

Corollary 3.2.3. *We have $\sigma(H_0) = \sigma_{ac}(H_0) \cup \sigma_{pp}(H_0)$, where*

$$\sigma_{ac}(H_0) = \bigcup_{n \in \mathbb{N}_0} [v_l + n\omega, v_l + 4 + n\omega] \cup [v_r + n\omega, v_r + 4 + n\omega]$$

and

$$\sigma_{pp}(H_0) = \bigcup_{n \in \mathbb{N}_0} \{m\omega_0 + n\omega \,|\, 0 \leq m \leq d-1\}.$$

The eigenvectors are given by $\widetilde{g}(m,n) = e_m \otimes \Upsilon_n$, $0 \leq m \leq d-1$, $n \in \mathbb{N}_0$. The generalized eigenfunctions are given by $\widetilde{g}_j(\lambda, n) = g_j(\lambda - n\omega) \otimes \Upsilon_n$ for $\lambda \in \sigma_{ac}(H_0)$, $n \in \mathbb{N}_0$, $j \in \{l, r\}$.

Proof. It is well known (see e.g. [30]) that for two self-adjoint operators A on $\mathfrak{h}_A$ and B on $\mathfrak{h}_B$ with $\sigma_{sc}(A) = \sigma_{sc}(B) = \emptyset$, we have $\sigma_{sc}(A \otimes 1 + 1 \otimes B) = \emptyset$, as well as

$$\sigma_{ac}(A \otimes 1 + 1 \otimes B) = \big(\sigma_{ac}(A) + \sigma(B)\big) \cup \big(\sigma(A) + \sigma_{ac}(B)\big),$$

and

$$\sigma_{pp}(A \otimes 1 + 1 \otimes B) = \sigma_{pp}(A) + \sigma_{pp}(B).$$

Thus, the statement about the spectrum of H_0 follows with $A = h_0^{el}$ and $B = h^{ph}$ using Lemma 3.2.2 and the fact that h_S^{el} has eigenvectors $\{e_0, \ldots, e_{d-1}\}$ with eigenvalues $\{m\omega_0 \,|\, 0 \leq m \leq d-1\}$. Furthermore, it is obvious that

$$H_0(e_m \otimes \Upsilon_n) = (h_0^{el} e_m) \otimes \Upsilon_n + e_m \otimes (h^{ph} \Upsilon_n) = (m\omega_0 + n\omega) e_m \otimes \Upsilon_n$$

for $0 \leq m \leq d-1$ and $n \in \mathbb{N}_0$. Finally, $\widetilde{g}_j(\lambda - n\omega)$ is bounded as an anti-linear functional on $\mathfrak{h}_j^{el} \otimes \mathfrak{h}^{ph}$ and satisfies

$$\langle \widetilde{g}_j(\lambda, n), H_0 f \rangle = \langle (\lambda - n\omega + n\omega) \widetilde{g}_j(\lambda, n), f \rangle = \lambda \langle \widetilde{g}_j(\lambda, n), f \rangle, \qquad f \in \mathrm{dom}(H_0),$$

in this sense. We refer to [32] for details on generalized eigenvectors. □

For $j \in \{l, r\}$ the generalized eigenfunctions of h_j^{el} give us the generalized Fourier transform $\phi_j^{el} : \ell^2(\mathbb{N}) \to L^2((v_j, v_j + 4))$ defined by

$$(\phi_j^{el} f)(\lambda) = \sum_{x \in \mathbb{N}} g_j(x, \lambda) f(x). \tag{3.27}$$

It is a spectral representation of h_j^{el} with

$$\mathfrak{h}_j^{el}(\lambda) = \begin{cases} \mathbb{C} & \text{if } \lambda \in (v_j, v_j + 4), \\ \{0\} & \text{if } \lambda \in \mathbb{R} \setminus (v_j, v_j + 4). \end{cases}$$

For $\lambda \in \mathbb{R}$ we define

$$\mathfrak{h}(\lambda) = \bigoplus_{n \in \mathbb{N}_0} \mathfrak{h}_n(\lambda), \qquad \mathfrak{h}_n(\lambda) = \mathfrak{h}^{el}(\lambda - n\omega),$$

where $\mathfrak{h}^{el}(\lambda) = \mathfrak{h}_l^{el}(\lambda) \oplus \mathfrak{h}_r^{el}(\lambda)$. For $j \in \{l, r\}$ we have $\mathfrak{h}_j^{el}(\lambda - n\omega) = \{0\}$ if the photon number n satisfies $\omega^{-1}(\lambda - v_j) \leq n \leq \omega^{-1}(\lambda - v_j - 4)$, whence $\dim(\mathfrak{h}(\lambda)) < \infty$ uniformly for a.e. $\lambda \in \mathbb{R}$. Note that $\mathfrak{H}_{H_0}^{ac} = \ell^2(\mathbb{N}_0, \mathfrak{h}_l^{el} \oplus \mathfrak{h}_r^{el})$ with

$$H_0^{ac}\{(f_l(n), f_r(n))\}_{n \in \mathbb{N}_0} = \{((h_l^{el} + n\omega) f_l(n), (h_r^{el} + n\omega) f_r(n))\}_{n \in \mathbb{N}_0},$$

whence a spectral representation $\Phi : \mathfrak{H}_{H_0}^{ac} \to L^2(\mathbb{R}, \mathrm{d}\lambda, \mathfrak{h}(\lambda))$ of H_0^{ac} is given by

$$(\Phi f)(\lambda) = \{((\phi_l^{el} f_l(n))(\lambda - n\omega), (\phi_r^{el} f_r(n))(\lambda - n\omega))\}_{n \in \mathbb{N}_0}$$

for $f = \{(f_l(n), f_r(n))\}_{n \in \mathbb{N}_0} \in \ell^2(\mathbb{N}_0, \mathfrak{h}_l^{el} \oplus \mathfrak{h}_r^{el})$, $\lambda \in \sigma(H_0^{ac})$, where ϕ_j^{el}, $j \in \{l, r\}$ are given by (3.27).

We now have full information on the spectral properties of H_0. We can use this to show that H has no singular continuous spectrum with the help of [9, Cor. IV.15.19], which establishes existence and completeness of wave operators and absence of singular continuous spectrum through a time-falloff method. We cite it as a Lemma for convenience, with slight simplifications that suffice for our purpose.

Lemma 3.2.4. *Let $\{H_0, H\}$ be a scattering system and let Γ be a closed countable set. Let F_+ and F_- be two self-adjoint operators such that $F_+ + F_- = P_{H_0}^{ac}$ and*

$$\operatorname*{s-lim}_{t \to \infty} e^{\mp itH_0} F_\pm e^{\pm itH_0} = 0.$$

If $(H - i)^{-1} - (H_0 - i)^{-1} \in \mathfrak{L}_\infty(\mathfrak{H})$, $(1 - P_{H_0}^{ac})\gamma(H_0) \in \mathfrak{L}_\infty(\mathfrak{H})$, and

$$\Big| \int_0^{\pm\infty} \mathrm{d}t \big\| ((H_0 - i)^{-1} - (H - i)^{-1}) e^{-itH_0} \gamma(H_0) F_\pm \big\| \Big| < \infty$$

for all $\gamma \in C_0^\infty(\mathbb{R} \setminus \Gamma)$, then the wave operators $W_\pm(H, H_0)$ exist and are complete and $\sigma_{sc}(H) = \sigma_{sc}(H_0) = \emptyset$. Furthermore, each eigenvalue of H and H_0 in $\mathbb{R} \setminus \Gamma$ is of finite multiplicity and these eigenvalues accumulate at most at points of Γ or at $\pm\infty$.

We already know that the wave operators exist and are complete since the resolvent difference is even trace class in our case. Hence, we need Lemma 3.2.4 only to prove the following proposition.

Proposition 3.2.5. *We have $\sigma_{sc}(H) = \emptyset$. Furthermore, the eigenvalues of H in $\mathbb{R} \setminus \Gamma$ are of finite multiplicity and accumulate at most at Γ or at $\pm\infty$, where*

$$\Gamma = \bigcup_{n\in\mathbb{N}_0} \{v_l + n\omega, v_r + n\omega, v_l + 4 + n\omega, v_r + 4 + n\omega\}.$$

Proof. First we have to construct the operators $F_\pm$. To this end, let $\Psi : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ be the usual Fourier transform. Further, let $\Pi_\pm$ be the orthogonal projection of $L^2(\mathbb{R})$ onto $L^2(\mathbb{R}_\pm)$. By continuation with zero we can consider every function $f \in L^2(\sigma_{ac}(H_0))$ as a function in $L^2(\mathbb{R})$ and vice versa by projection. In this sense we can define

$$F_\pm = \Phi^*\Psi\Pi_\pm\Psi^*\Phi,$$

where Φ is the spectral representation of H_0^{ac} constructed above. We immediately obtain $F_- + F_+ = P_{H_0}^{ac}$. We still have to show that

$$\lim_{t\to\infty} \|e^{\mp itH_0}\Phi^*\Psi\Pi_\pm\Psi^*\Phi e^{\pm itH_0} f\| = 0$$

for $f \in \mathfrak{H}_{H_0}^{ac}$. We prove the relation only for F_+ since the proof for F_- is essentially identical. We have

$$(\Pi_+\Psi^*\Phi e^{itH_0} f)(x) = (2\pi)^{-\frac{1}{2}}\chi_{[0,\infty)}(x)\int_{\mathbb{R}} \mathrm{d}\mu\, e^{i(x+t)\mu}\widehat{f}(\mu) = \chi_{[0,\infty)}(x)\psi(x+t)$$

with $\psi = \Psi\widehat{f}$. Now

$$\begin{aligned}\|e^{-itH_0}\Phi^*\Psi\Pi_+\Psi^*\Phi e^{itH_0} f\|^2 &= \|\Pi_+\Psi^*\Phi e^{itH_0} f\|^2 \\ &= \int_{\mathbb{R}} \mathrm{d}y |\chi_{[0,\infty)}(y-t)\psi(y)|^2 \\ &= \int_t^\infty \mathrm{d}y |\psi(y)|^2 \overset{t\to\infty}{\longrightarrow} 0.\end{aligned}$$

We already know that $(H-i)^{-1} - (H_0-i)^{-1} \in \mathfrak{L}_1(\mathfrak{H}) \subset \mathfrak{L}_\infty(\mathfrak{H})$ from Proposition 3.2.1. Let

$$\Gamma = \bigcup_{n\in\mathbb{N}_0} \{v_l + n\omega, v_r + n\omega, v_l + 4 + n\omega, v_r + 4 + n\omega\},$$

which is closed and countable. We know from Corollary 3.2.3 that H_0 has no singular continuous spectrum and the eigenvalues are of finite multiplicity. It follows that the operator $(1 - P_{ac}(H_0))\gamma(H_0)$ is compact for every $\gamma \in C_0^\infty(\mathbb{R} \setminus \Gamma)$. The remaining assumption of Lemma 3.2.4 is

$$\Big| \int_0^{\pm\infty} \mathrm{d}t \, \big\|((H-i)^{-1} - (H_0-i)^{-1})\gamma(H_0)e^{-itH_0}F_\pm\big\| \Big| < \infty.$$

If we can prove this, we immediately obtain the statement of the proposition. Note that

$(H-i)^{-1}-(H_0-i)^{-1}=(H-i)^{-1}(V_{el}+V_{int})(H_0-i)^{-1}$. But $(H-i)^{-1}$ is bounded,

$$\mathrm{ran}(F_\pm)\subset\mathfrak{H}^{ac}_{H_0}=(\mathfrak{h}^{el}_l\oplus\mathfrak{h}^{el}_r)\otimes\mathfrak{h}^{ph},$$

and $V_{int}P^{ac}_{H_0}=0$. Also, $V_{el}=v_{el}\otimes I_{ph}$ and $\ker(v_{el})^\perp\subset\mathbb{C}x^1_l\oplus\mathfrak{h}^{el}_S\oplus\mathbb{C}x^1_r$. Hence, it suffices to prove

$$\Big|\int_0^{\pm\infty}\mathrm{d}t\,\|P^j_1(H_0-i)^{-1}\gamma(H_0)e^{-itH_0}\Phi^*\Psi f\|\Big|<\gamma_j\|f\|$$

for any $f\in L^2(\mathbb{R})$ with $\mathrm{supp}(f)\subset\mathbb{R}_\pm$ and $j\in\{l,r\}$, where $P^j_1=p^j_1\otimes I_{ph}$ and p^j_1 is the orthogonal projection onto $\mathbb{C}x^1_j$. In the following we treat only the case F_+. The calculations for F_- are completely analogous. Using the fact that Φ maps H^{ac}_0 into the multiplication operator $\mathcal{M}(\lambda)$ and that the Fourier transform maps the unitary group $e^{-it\mathcal{M}(\lambda)}$ into the translation by t, we obtain

$$\begin{aligned}
&\int_0^\infty\mathrm{d}t\,\|P^j_1(H_0-i)^{-1}\gamma(H_0)e^{-itH_0}\Phi^*\Psi f\|\\
&\quad=\int_0^\infty\mathrm{d}t\,\|P^j_1\Phi^*\Phi(H_0-i)^{-1}\gamma(H_0)e^{-itH_0}\Phi^*\Psi f\|\\
&\quad=(2\pi)^{-\frac12}\int_0^\infty\mathrm{d}t\Big(\sum_{n\in\mathbb{N}_0}\int_{v_j+n\omega}^{v_j+4+n\omega}\mathrm{d}\lambda\,\Big|w_j(\lambda,n)\int_{\mathbb{R}}\mathrm{d}y\,e^{-i\lambda y}\widehat{f}(y-t)\Big|^2\Big)^{\frac12}
\end{aligned}$$

with $w_j(\lambda,n)=g_j(1,\lambda-n\omega)(\lambda-i)^{-1}\gamma(\lambda)$. It is obvious from the definition that the integral is finite on $(0,\widetilde{\gamma})$ for some $\widetilde{\gamma}>0$. It remains to estimate

$$\begin{aligned}
&\int_{\widetilde{\gamma}}^\infty\mathrm{d}t\Big(\sum_{n\in\mathbb{N}_0}\int_{v_j+n\omega}^{v_j+4+n\omega}\mathrm{d}\lambda\,\Big|w_j(\lambda,n)\int_{\mathbb{R}}\mathrm{d}y\,e^{-i\lambda y}\widehat{f}(y-t)\Big|^2\Big)^{\frac12}\\
&\quad\le\int_{\widetilde{\gamma}}^\infty\mathrm{d}t\sum_{n\in\mathbb{N}_0}\int_{v_j+n\omega}^{v_j+4+n\omega}\mathrm{d}\lambda\,\Big|\Big(\frac{\mathrm{d}^4}{\mathrm{d}\lambda^4}w_j(\lambda,n)\Big)\int_{\mathbb{R}}\mathrm{d}y\,(-iy)^{-4}e^{-i\lambda y}\widehat{f}(y-t)\Big|,
\end{aligned}$$

where we integrated partially four times. This is possible because γ is smooth with compact support away from $v_r+n\omega$ and $v_r+n\omega+4$ and $g_j(1,\lambda-n\omega)$ is smooth for $\lambda\in(v_r+n\omega,v_r+n\omega+4)$, $n\in\mathbb{N}_0$. Now we use that y^{-2} is decreasing on (t,∞) for $t>0$ and $\widehat{f}$ has support in $\mathbb{R}_+$. Also note that $\beta(y)=(y+t)^{-2}$ is in $L^2((t,\infty))$ for $t>0$. It follows that

$$\begin{aligned}
&\int_{\widetilde{\gamma}}^\infty\mathrm{d}t\sum_{n\in\mathbb{N}_0}\int_{v_j+n\omega}^{v_j+4+n\omega}\mathrm{d}\lambda\,\Big|\Big(\frac{\mathrm{d}^4}{\mathrm{d}\lambda^4}w_j(\lambda,n)\Big)\int_{\mathbb{R}}\mathrm{d}y\,(-iy)^{-4}e^{-i\lambda y}\widehat{f}(y-t)\Big|\\
&\quad\le\int_{\widetilde{\gamma}}^\infty\mathrm{d}t\sum_{n\in\mathbb{N}_0}\int_{v_j+n\omega}^{v_j+4+n\omega}\mathrm{d}\lambda\,t^{-2}\Big|\frac{\mathrm{d}^4}{\mathrm{d}\lambda^4}w_j(\lambda,n)\Big|\int_{\mathbb{R}}\mathrm{d}y\,|y^{-2}\widehat{f}(y-t)|\\
&\quad\le\int_{\widetilde{\gamma}}^\infty\mathrm{d}t\,t^{-2}\sum_{n\in\mathbb{N}_0}\int_{v_j}^{v_j+4}\mathrm{d}\nu\,\Big|\frac{\mathrm{d}^4}{\mathrm{d}\nu^4}w_j(\nu+n\omega,n)\Big|\,\|\beta\|\,\|\widehat{f}\|\\
&\quad\le\widetilde{\alpha}\|\widehat{f}\|
\end{aligned}$$

for some $\widetilde{\alpha}>0$. For the final estimate in the above inequality, note that the derivative

has compact support, whence the integral over ν is finite for every $n \in \mathbb{N}_0$. But the compact support implies that the sum over n is actually finite. With this estimate and a similar one for F_-, the proposition follows from Lemma 3.2.4. □

Proposition 3.2.1 together with Corollary 3.2.3 and Proposition 3.2.5 shows that H_0 and H satisfy assumption (A1) in Section 3.1.2. Thus, we obtain a Landauer-Büttiker formula if we choose an initial state ρ_0 and an observable Q satisfying (A3) respectively (A2).

Recall that in the purely electric case, the trace in the Landauer-Büttiker formula for the current reduced to the scattering cross-section $\sigma^{el}_{lr}(\lambda)$, cf. Section 3.1.1. We can define similar quantities for the scattering system $\{H_0, H\}$.

Definition 3.2.6. *Let $j,k \in \{l,r\}$ and $m,n \in \mathbb{N}_0$ and let $P_{j,n}(\lambda)$ denote the orthogonal projection of $\mathfrak{h}(\lambda)$ onto $\mathfrak{h}^{el}_j(\lambda - n\omega)$. Then the* channel cross-section *between channels (j,n) and (k,m) is defined by*

$$\sigma_{jk,nm}(\lambda) = \operatorname{Tr}\big(T^*_{jk,nm}(\lambda)T_{jk,nm}(\lambda)\big),$$

where the channel transition matrices are given by $T_{jk,nm}(\lambda) = P_{j,n}(\lambda)T(\lambda)P_{k,m}(\lambda)$. Furthermore, we define the electron channel cross-section

$$\sigma_{jk}(\lambda) = \operatorname{Tr}\big(T^*_{jk}(\lambda)T_{jk}(\lambda)\big),$$

where the electron channel transition matrices are given by $T_{jk}(\lambda) = P_j(\lambda)T(\lambda)P_k(\lambda)$ and $P_j(\lambda)$ is the orthogonal projection onto $\bigoplus_{n\in\mathbb{N}_0}\mathfrak{h}^{el}_j(\lambda - n\omega)$ in $\mathfrak{h}(\lambda)$.

Lemma 3.2.7. *Let $j,k \in \{l,r\}$ and $m,n \in \mathbb{N}_0$. For a.e. $\lambda \in \mathbb{R}$, the channel cross-section $\sigma_{jk,nm}(\lambda)$ satisfies*

$$\sum_{k\in\{l,r\}}\sum_{m\in\mathbb{N}_0}\sigma_{jk,nm}(\lambda) = \sum_{k\in\{l,r\}}\sum_{m\in\mathbb{N}_0}\sigma_{kj,mn}(\lambda). \tag{3.28}$$

Furthermore, the electron channel cross-section σ_{lr} satisfies

$$\sigma_{lr}(\lambda) = \sum_{m,n\in\mathbb{N}_0}\sigma_{lr,nm}(\lambda) = \sum_{m,n\in\mathbb{N}_0}\sigma_{rl,nm}(\lambda) = \sigma_{rl}(\lambda).$$

Proof. Note that T is a normal operator since $S^*S = P^{ac}_{H_0}$ implies

$$(2\pi)^{-2}T^*T = (P^{ac}_{H_0} - S^*)(P^{ac}_{H_0} - S) = 2P^{ac}_{H_0} - S^* - S = (2\pi)^{-2}TT^*.$$

Furthermore, $\sum_{k\in\{l,r\}}\sum_{m\in\mathbb{N}_0}P_{k,m}(\lambda) = I_{\mathfrak{h}(\lambda)}$, whence, using the cyclicity of the trace,

$$\begin{aligned}\sum_{k\in\{l,r\}}\sum_{m\in\mathbb{N}_0}\operatorname{Tr}\big(T^*_{jk,nm}(\lambda)T_{jk,nm}(\lambda)\big) &= \operatorname{Tr}\big(P_{j,n}(\lambda)T^*(\lambda)T(\lambda)\big)\\ &= \sum_{k\in\{l,r\}}\sum_{m\in\mathbb{N}_0}\operatorname{Tr}\big(P_{k,m}(\lambda)T^*(\lambda)P_{j,n}(\lambda)T(\lambda)\big)\\ &= \sum_{k\in\{l,r\}}\sum_{m\in\mathbb{N}_0}\sigma_{kj,nm}(\lambda).\end{aligned}$$

Obviously, it follows that

$$\sigma_{ll}(\lambda)+\sigma_{lr}(\lambda)=\sum_{k\in\{l,r\}}\sum_{m,n\in\mathbb{N}_0}\sigma_{lk,nm}(\lambda)=\sum_{k\in\{l,r\}}\sum_{m,n\in\mathbb{N}_0}\sigma_{kl,mn}(\lambda)=\sigma_{ll}(\lambda)+\sigma_{rl}(\lambda),$$

which concludes the proof of the lemma. □

A time-reversal symmetric two-level quantum dot

Before we state the Landauer-Büttiker formula for the Jaynes-Cummings QD-LED, we present a special choice for the Hamiltonian of the quantum dot. Namely, let $d=2$ and choose h_S^{el} such that

$$e_0=\frac{1}{\sqrt{2}}(x_S^0+x_S^1)\qquad\text{and}\qquad e_1=\frac{1}{\sqrt{2}}(x_S^0-x_S^1). \tag{3.29}$$

This system has the special property of being time-reversal symmetric.

Definition 3.2.8. *A scattering system $\{H_0,H\}$ is called* time-reversal symmetric *if there exists a conjugation ι, i.e. a bounded anti-linear operator ι on $\mathfrak{H}$ such that $\iota^2=I_{\mathfrak{H}}$ and $\langle \iota f,\iota g\rangle=\overline{\langle f,g\rangle}$ for $f,g\in\mathfrak{H}$, that commutes with H_0 and H simultaneously*

Proposition 3.2.9. *The two-level QD-LED model given by* (3.29) *is time-reversal symmetric.*

Proof. Define the conjugation $\iota^{el}=\iota_l^{el}\oplus\iota_S^{el}\oplus\iota_r^{el}$ by

$$(\iota_j^{el}f_j^{el})(x)=\overline{f_j^{el}(x)},\qquad x\in\mathbb{N},\qquad (\iota_S^{el}f_S^{el})(x)=\overline{f_S^{el}(x)},\qquad x\in\{0,1\},$$

for $j\in\{l,r\}$. Obviously, for $j\in\{l,r\}$ and $f_j^{el}\in\mathfrak{h}_j^{el}$, we have

$$(\iota_j^{el}h_j^{el}f_j^{el})(x)=\overline{-f_j^{el}(x+1)+(2+v_j)f_j^{el}(x)+f_j^{el}(x-1)}=(h_j^{el}\iota_j^{el}f_j^{el})(x).$$

Also, (3.29) implies

$$\iota_S^{el}e_0=\iota_S^{el}\tfrac{1}{\sqrt{2}}(x_S^0+x_S^1)=e_0,\qquad \iota_S^{el}e_1=\iota_S^{el}\tfrac{1}{\sqrt{2}}(x_S^0-x_S^1)=e_1$$

Thus,

$$\iota_S^{el}h_S^{el}e_m=\lambda_m\iota_S^{el}e_m=h_S^{el}e_m=h_S^{el}\iota_S^{el}e_m,\qquad m\in\{0,1\}.$$

It follows that ι^{el} commutes with h_0^{el}. Note that

$$\mathrm{ran}(v_{el})=\ker(v_{el})^{\perp}=\mathrm{span}\{x_l^1,x_S^0,x_S^1,x_r^1\}.$$

Let $f^{el}=(f_l^{el},f_S^{el}(0),f_S^{el}(1),f_r^{el})\in\ker(v_{el})^{\perp}$. We obtain

$$\iota_{el}v_{el}f^{el}=(\overline{f_S^{el}(0)},\overline{f_l^{el}},\overline{f_r^{el}},\overline{f_S^{el}(1)})=v_{el}\iota^{el}f^{el}.$$

Thus, ι^{el} commutes also with $h^{el}=h_0^{el}+\tau_{el}v_{el}$. Define the conjugation ι^{ph} on $\mathfrak{h}^{ph}$ by

$$(\iota^{ph}f^{ph})(n)=\overline{f^{ph}(n)},\qquad n\in\mathbb{N}_0.$$

Obviously, $(\iota^{ph}h^{ph}f^{ph})(n) = n\omega(\iota^{ph}f^{ph})(n)$, whence ι^{ph} commutes with h^{ph}. It follows that the conjugation $\iota = \iota^{el}\otimes\iota^{ph}$ commutes with H_0. It remains to check that ι commutes with V_{int} and thus with H. Let $f_S = \{(f_{S,n}(0), f_{S,n}(1))\}_{n\in\mathbb{N}_0} \in \mathfrak{h}_S^{el}\otimes\mathfrak{h}^{ph}$ with respect to $\{e_0\otimes\Upsilon_n, e_1\otimes\Upsilon_n\}_{n\in\mathbb{N}_0}$. We obtain from $\iota_S^{el}e_m = e_m$, $m\in\{0,1\}$, and $\iota^{ph}\Upsilon_n = \Upsilon_n$, $n\in\mathbb{N}_0$, that

$$\iota(V_{int}f_S) = \{(\overline{f_{S,n-1}(1)}, \overline{f_{S,n+1}(0)})\}_{n\in\mathbb{N}_0} = V_{int}\{(\overline{f_{S,n}(0)}, \overline{f_{S,n}(1)})\}_{n\in\mathbb{N}_0} = V_{int}(\iota f_S),$$

where we define $f_{S,-1} = 0$. Hence, the proposition follows. □

The time-reversal symmetry gives us a symmetry in the transition matrix.

Proposition 3.2.10. *The transition matrix of the two-level QD-LED model given by* (3.29) *satisfies* $\sigma_{jk,nm}(\lambda) = \sigma_{kj,mn}(\lambda)$ *for* $j,k\in\{l,r\}$ *and* $n,m\in\mathbb{N}_0$.

Proof. Note that the conjugation ι commutes with $P_{j,n}$ for $j\in\{l,r\}$ and $n\in\mathbb{N}_0$. Also, it is well-known that $\iota W_\pm(H,H_0) = W_\mp(H,H_0)\iota$, which implies

$$\iota S = W_-^*(H,H_0)W_+(H,H_0)\iota = S^*\iota.$$

Furthermore, ι commutes with H_0, whence a spectral representation of H_0^{ac} maps it to a multiplication operator $\mathcal{M}(\iota(\lambda)) = \Phi_{H_0}\iota\Phi_{H_0}^*$ such that $\iota(\lambda)$ is a conjugation on $\mathfrak{h}(\lambda)$. From this we obtain

$$\iota(\lambda)T^*(\lambda)T(\lambda) = T(\lambda)T^*(\lambda)\iota(\lambda),$$

Let $j,k\in\{l,r\}$ and $n,m\in\mathbb{N}_0$. We have $\sigma_{jk,nm}(\lambda)\geq 0$. Furthermore, let $\{\widehat{g}_{\nu_1}\}_{\nu_1\in\mathbb{N}}$ be a basis of $\mathfrak{h}(\lambda)$. For a trace class operator $Z\in\mathfrak{L}_1(\mathfrak{h}(\lambda))$ with $Z = \sum_{\nu_2\in\mathbb{N}}\zeta_{\nu_2}\langle z_{\nu_2},\cdot\rangle z_{\nu_2}$ with $\|z_{\nu_2}\| = 1$, $\nu_2\in\mathbb{N}$, we use the anti-linearity of $\iota(\lambda)$ to obtain

$$\begin{aligned}
\mathrm{Tr}(\iota(\lambda)Z\iota(\lambda)) &= \sum_{\nu_1,\nu_2\in\mathbb{N}}\overline{\zeta_{\nu_2}}\langle\widehat{g}_{\nu_1},\iota(\lambda)z_{\nu_2}\rangle\overline{\langle z_{\nu_2},\iota(\lambda)\widehat{g}_{\nu_1}\rangle}\\
&= \sum_{\nu_1,\nu_2\in\mathbb{N}}\overline{\zeta_{\nu_2}}\langle\widehat{g}_{\nu_1},\iota(\lambda)z_{\nu_2}\rangle\langle\iota(\lambda)z_{\nu_2},\widehat{g}_{\nu_1}\rangle\\
&= \sum_{\nu_2\in\mathbb{N}}\overline{\zeta_{\nu_2}}\|z_{\nu_2}\|^2\\
&= \overline{\mathrm{Tr}(Z)}.
\end{aligned}$$

It follows that

$$\begin{aligned}
\sigma_{jk,nm}(\lambda) &= \overline{\mathrm{Tr}(T_{jk,nm}^*(\lambda)T_{jk,nm}(\lambda))}\\
&= \mathrm{Tr}(\iota(\lambda)P_{k,m}(\lambda)T^*(\lambda)P_{j,n}(\lambda)T(\lambda)P_{k,m}(\lambda)\iota(\lambda))\\
&= \mathrm{Tr}(T_{kj,mn}(\lambda)T_{kj,mn}^*(\lambda))\\
&= \sigma_{kj,mn}(\lambda).
\end{aligned}$$

□

In the special case of $v_l = v_r$, we obtain a system that is mirror symmetric.

Proposition 3.2.11. *Let the two-level QD-LED model given by* (3.29) *satisfy* $v_l = v_r$. *Then it is a mirror symmetric system, i.e. there is a unitary operator* U *satisfying* $UH_S = H_S U$ *and* $UH_j = H_k U$ *for* $j,k \in \{l,r\}$, $j \neq k$.

Proof. Define $u^{el}_{lr} \in \mathfrak{B}(\mathfrak{h}^{el}_l \oplus \mathfrak{h}^{el}_r)$ by $u^{el}_{lr}(f^{el}_l, f^{el}_r) = (f^{el}_r, f^{el}_l)$. Obviously, since $v_l = v_r$, we have $h^{el}_j u^{el}_{lr} = u^{el}_{lr} h^{el}_k$ for $j,k \in \{l,r\}$, $j \neq k$. Furthermore, define the unitary operator $u^{el}_S \in \mathfrak{B}(\mathfrak{h}^{el}_S)$ by $u^{el}_S e_0 = e_0$ and $u^{el}_S e_1 = -e_1$. This gives us $h^{el}_S u^{el}_S = u^{el}_S h^{el}_S$. Since $x^0_S = \frac{1}{\sqrt{2}}(e_0 + e_1)$ and $x^1_S = \frac{1}{\sqrt{2}}(e_0 - e_1)$, we have $u^{el}_S x^0_S = x^1_S$ and $u^{el}_S x^1_S = x^0_S$. Now we set $u^{el} = u^{el}_l \oplus u^{el}_S \oplus u^{el}_r$. Note that $\mathrm{ran}(v_{el}) = \ker(v_{el})^\perp = \mathrm{span}\{x^1_l, x^0_S, x^1_S, x^1_r\}$. Let $f^{el} = (f^{el}_l, f^{el}_S(0), f^{el}_S(1), f^{el}_r) \in \ker(v_{el})^\perp$. We obtain

$$\begin{aligned} u^{el} v_{el} f^{el} = u^{el}(f^{el}_S(0), f^{el}_l, f^{el}_r, f^{el}_S(1)) &= (f^{el}_S(1), f^{el}_r, f^{el}_l, f^{el}_S(0) x^1_r) \\ &= v_{el}(f^{el}_r, f^{el}_S(1), f^{el}_l(0), f^{el}_l) = v_{el} u^{el} f. \end{aligned}$$

The unitary operator on $\mathfrak{h}^{ph}$ is given by $u^{ph} f^{ph} = (-1)^n f^{ph}$. We define $U = u^{el} \otimes u^{ph}$, which implies $UV_{el} = V_{el} U$ for $V_{el} = v_{el} \otimes I_{ph}$. For $f_S = \{(f_{S,n}(0), f_{S,n}(1))\}_{n \in \mathbb{N}_0}$ with respect to $\bigcup_{n \in \mathbb{N}_0} \{e_0 \otimes \Upsilon_n, e_1 \otimes \Upsilon_n\}$, we get

$$\begin{aligned} UV_{int}(f_l, f_S, f_r) &= U\big(f_l, \{(f_{S,n-1}(1), f_{S,n+1}(0))\}_{n \in \mathbb{N}_0}, f_r\big) \\ &= \big(f_r, \{(-1)^n (f_{S,n-1}(1), -f_{S,n+1}(0))\}_{n \in \mathbb{N}_0}, f_l\big) \\ &= V_{int}\big(f_r, \{((-1)^n f_{S,n}(0), -(-1)^n f_{S,n}(1))\}_{n \in \mathbb{N}_0}, f_l\big) \\ &= V_{int} U\big(f_l, \{(f_{S,n}(0), f_{S,n}(1))\}_{n \in \mathbb{N}_0}, f_r\big), \end{aligned}$$

where we define $f_{S,-1} = 0$. □

This mirror symmetry gives us another symmetry for the channel cross section.

Proposition 3.2.12. *Let the two-level QD-LED model given by* (3.29) *satisfy* $v_l = v_r$. *Then* $\sigma_{jk,nm}(\lambda) = \sigma_{kj,nm}(\lambda)$ *for all* $j,k \in \{l,r\}$ *and* $n,m \in \mathbb{N}_0$.

Proof. Let $j,k \in \{l,r\}$ and $n,m \in \mathbb{N}_0$. The claim of the proposition is trivial for $j = k$. Let $j \neq k$ and U be given as in the proof of Proposition 3.2.11. Then $[U, H_0] = 0$ and $UP_{j,n} = P_{k,n} U$. Furthermore, $[U, W_\pm(H, H_0)] = 0$, which implies $[U, T] = 0$. We obtain

$$\begin{aligned} \sigma_{jk,nm}(\lambda) &= \mathrm{Tr}\big(U(\lambda) P_{k,m}(\lambda) T^*(\lambda) P_{j,n}(\lambda) T(\lambda) P_{k,m}(\lambda) U^*(\lambda)\big) \\ &= \mathrm{Tr}\big(P_{j,m}(\lambda) T^*(\lambda) P_{k,n}(\lambda) T(\lambda) P_{kj,m}(\lambda)\big) \\ &= \sigma_{kj,nm}(\lambda), \end{aligned}$$

where $U(\lambda)$ is given by $\Phi_{H_0} U \Phi^*_{H_0} = \mathcal{M}(U(\lambda))$ since U commutes with H_0. □

3.2.2 The Landauer-Büttiker formula

Just like the decoupled Hamiltonian H_0, the initial state ρ_0 of the decoupled system is not unique, and in general different initial states result in different final steady states. For ρ_0 to be a reasonable initial state for fermions, it should at least satisfy $0 \leq \rho_0 \leq 1$, cf. Equation (A.1.8) in the appendix. In the case of the QD-LED, there are two physically obvious choices for ρ_0. In both cases the basic assumption is that the leads and the

quantum dot are separately in equilibrium, analogously to the purely electric model. However, it is not immediately obvious what this means. One possible approach is to use the picture of non-interacting fermions. Recall that we treat an electron together with its photon field as a non-interacting particle. But the equilibrium state of non-interacting fermions is given by the Fermi-Dirac distribution function, whence a natural choice for the initial state is

$$\rho_0 = \rho_l \oplus \rho_S \oplus \rho_r, \qquad \rho_j = f_{FD}(H_j - \mu_j), \qquad f_{FD}(\lambda) = (1 + e^{\beta\lambda})^{-1}, \tag{3.30}$$

where $j \in \{l, S, r\}$. Here, μ_j are the chemical potentials in the leads, and $\beta > 0$ is the inverse temperature. One could choose different temperatures in the subsystems, but we are not interested in the heat flux of the system, whence we choose a global temperature for all subsystems. Note that $\rho_0 = f_{FD}(H_0 - \mu)$ is an equilibrium state for the total system if the chemical potentials in all subsystems are equal, i.e. $\mu = \mu_j$ for all $j \in \{l, S, r\}$. Corollary 3.1.3 implies that all fluxes are zero in this case. Also, recall that the state of the quantum dot has no effect on the steady state flux since the spectrum of H_S is pure point.

A second approach to defining the initial state is to assume that the electrons in every subsystem are in equilibrium and the photon field is also in equilibrium. Then we have

$$\widetilde{\rho}_0^{el} = f_{FD}(h_l^{el} - \mu_l) \oplus f_{FD}(h_S^{el} - \mu_S) \oplus f_{FD}(h_r^{el} - \mu_r)$$

for the electrons. For the photons we take the Gibbs grand canonical equilibrium state

$$\widetilde{\rho}_0^{ph} = \frac{1}{\mathrm{Tr}(e^{-\beta h^{ph}})} e^{-\beta h^{ph}} = (1 - e^{-\beta\omega}) e^{-\beta h^{ph}},$$

cf. (A.1.10) in the appendix. The initial state is then $\widetilde{\rho}_0 = \widetilde{\rho}_0^{el} \otimes \widetilde{\rho}_0^{ph}$. Note that this is a steady state, i.e. $[H_0, \rho_0] = 0$, but even if all chemical potentials are equal, it is not an equilibrium state since it can not be written as a function of H_0.

Both ρ_0 and $\widetilde{\rho}_0$ satisfy Assumption (A3) for any $N_{max} \in \mathbb{N}$ due to the exponential decay in the photon energy. Thus, the following theorem about the electron current and the photon production rate immediately follows from the Landauer-Büttiker formula of Theorem 3.1.2. Recall that p_j^{el} is the orthogonal projection onto $\mathfrak{h}_j^{el}$ and $\mathfrak{N}_+$ is the number operator on $\mathfrak{F}_+(\mathbb{C})$.

Theorem 3.2.13. *Let Q satisfy Assumption* (A2)*. The flux of Q with respect to the initial states ρ_0 and $\widetilde{\rho}_0$ is given by*

$$\mathfrak{J}_{Q,\rho_0} = \frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{d}\lambda \mathrm{Tr}\Big(\rho_0(\lambda)(S^*(\lambda)Q(\lambda)S(\lambda) - Q(\lambda))\Big)$$

and

$$\mathfrak{J}_{Q,\widetilde{\rho}_0} = \frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{d}\lambda \mathrm{Tr}\Big(\widetilde{\rho}_0(\lambda)(S^*(\lambda)Q(\lambda)S(\lambda) - Q(\lambda))\Big).$$

In particular, $Q = -p_j^{el} \otimes I_{ph}$ gives the electron current out of lead j, $j \in \{l, r\}$, and $Q = I_{el} \otimes \mathfrak{N}_+$ gives the photon production rate.

In the following, we analyze $\mathfrak{J}_{Q,\rho_0}$ and $\mathfrak{J}_{Q,\widetilde{\rho}_0}$, in particular for the electron current

and the photon production rate. To obtain the individual contributions of the coupling of the leads and the electron-photon interaction, respectively, we introduce the Hamiltonian H_{el}, describing the quantum system with coupled leads but no electron-photon interaction. It is given by

$$H_{el} = H_0 + \tau_{el} V_{el}, \qquad \mathrm{dom}(H_{el}) = \mathrm{dom}(H_0). \tag{3.31}$$

From the proof of Proposition 3.2.1 it is obvious that $(H_{el}+\theta)^{-1} - (H_0+\theta)^{-1} \in \mathfrak{L}_1(\mathfrak{H})$ and $(H+\theta)^{-1} - (H_{el}+\theta)^{-1} \in \mathfrak{L}_1(\mathfrak{H})$. This implies that we get Landauer-Büttiker formulae for the scattering systems $\{H_0, H_{el}\}$ and $\{H_{el}, H\}$ with scattering operators

$$S_{el} = W_+^*(H_{el}, H_0) W_-(H_{el}, H_0) \qquad \text{and} \qquad S_{ph} = W_+^*(H, H_{el}) W_-(H, H_{el}),$$

respectively. Define

$$Q_{el} = W_+(H_{el}, H_0) Q W_+^*(H_{el}, H_0), \qquad \rho_{el} = W_-(H_{el}, H_0) \rho_0 W_-^*(H_{el}, H_0). \tag{3.32}$$

Q_{el} and ρ_{el} satisfy Assumptions (A2) and (A3) with respect to H_{el}. Recall that we write

$$\Phi_{H_0} X_0 \Phi_{H_0}^* = \mathcal{M}(X_0(\lambda)) \qquad \text{and} \qquad \Phi_{H_{el}} X_{el} \Phi_{H_{el}}^* = \mathcal{M}(\widehat{X}_{el}(\lambda))$$

for spectral representations Φ_{H_0} of H_0^{ac} and $\Phi_{H_{el}}$ of H_{el}^{ac}, respectively, where X_0 and X_{el} are operators on $\mathfrak{H}$ commuting with H_0 respectively H_{el}. We obtain the following decomposition of the flux.

Proposition 3.2.14. *Let $\{H_0, H\}$ be the scattering system of the Jaynes-Cummings QD-LED, and let H_{el} be given by* (3.31)*. For any observable Q and any state ρ_0 satisfying Assumptions* (A2) *and* (A3)*, respectively, with $N, N_0, N_Q = 1$, the flux $\mathfrak{J}_{Q,\rho_0}$ decomposes into $\mathfrak{J}_{Q,\rho_0} = \mathfrak{J}^{el}_{Q,\rho_0} + \mathfrak{J}^{ph}_{Q,\rho_0}$, where*

$$\mathfrak{J}^{el}_{Q,\rho_0} = -i\,\mathrm{Tr}\Big(W_-(H_{el}, H_0)(H_0+\theta)^4 \rho_0 W_-^*(H_{el}, H_0)(H_{el}+\theta)^{-1} \\ \times \big[(H_{el}+\theta)^{-1} - (H_0+\theta)^{-1}, Q\big](H_{el}+\theta)^{-1}\Big)$$

is the contact-induced current and

$$\mathfrak{J}^{ph}_{Q,\rho_0} = -i\,\mathrm{Tr}\Big(W_-(H, H_{el})(H_{el}+\theta)^4 \rho_{el} W_-^*(H, H_{el})(H+\theta)^{-1} \\ \times \big[(H+\theta)^{-1} - (H_{el}+\theta)^{-1}, Q_{el}\big](H+\theta)^{-1}\Big)$$

is the photon-induced current. Furthermore,

$$\mathfrak{J}^{el}_{Q,\rho_0} = -\frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{d}\lambda\, \mathrm{Tr}\Big(\rho_0(\lambda)\big(Q(\lambda) - S_{el}^*(\lambda) Q(\lambda) S_{el}(\lambda)\big)\Big) \tag{3.33}$$

and

$$\mathfrak{J}^{ph}_{Q,\rho_0} = -\frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{d}\lambda\, \mathrm{Tr}\Big(\widehat{\rho}_{el}(\lambda)\big(\widehat{Q}_{el}(\lambda) - \widehat{S}_{ph}^*(\lambda) \widehat{Q}_{el}(\lambda) \widehat{S}_{ph}(\lambda)\big)\Big). \tag{3.34}$$

Proof. The representations (3.33) and (3.34) follow immediately from the Landauer-

Büttiker formula of Theorem 3.1.2. We use $S_{el} = W_+^*(H_{el}, H_0)W_-(H_{el}, H_0)$ with the wave matrices $\Phi_{H_{el}} W_\pm(H_{el}, H_0)\Phi_{H_0}^* = \mathcal{M}(W_\pm(\lambda))$ and the cyclicity of the trace to obtain

$$\begin{aligned}
&\mathrm{Tr}(\widehat{\rho}_{el}(\lambda)(\widehat{Q}_{el}(\lambda) - \widehat{S}_{ph}^*(\lambda)\widehat{Q}_{el}(\lambda)\widehat{S}_{ph}(\lambda))) \\
&\quad = \mathrm{Tr}\Big(W_-(\lambda)\rho_0(\lambda)W_-^*(\lambda)\Big(W_+(\lambda)Q(\lambda)W_+^*(\lambda) - S_{ph}^*(\lambda)W_+(\lambda)Q(\lambda)W_+^*(\lambda)S_{ph}(\lambda)\Big)\Big) \\
&\quad = \mathrm{Tr}\Big(\rho_0(\lambda)\Big(S_{el}^*(\lambda)Q(\lambda)S_{el}(\lambda) - W_-^*(\lambda)S_{ph}^*(\lambda)W_+(\lambda)Q(\lambda)W_+^*(\lambda)S_{ph}(\lambda)W_-(\lambda)\Big)\Big).
\end{aligned}$$

Since the chain rule for wave operators, Theorem A.2.11, gives us

$$W_\pm(H, H_0) = W_\pm(H, H_{el})W_\pm(H_{el}, H_0),$$

we obtain

$$S(\lambda) = W_+^*(\lambda)S_{ph}(\lambda)W_-(\lambda).$$

It follows that

$$\begin{aligned}
&\mathrm{Tr}(\widehat{\rho}_{el}(\lambda)(\widehat{Q}_{el}(\lambda) - \widehat{S}_{ph}^*(\lambda)\widehat{Q}_{el}(\lambda)\widehat{S}_{ph}(\lambda))) \\
&\quad = \mathrm{Tr}(\rho_0(\lambda)(S_{el}^*(\lambda)Q(\lambda)S_{el}(\lambda) - S(\lambda)Q(\lambda)S(\lambda))).
\end{aligned}$$

Adding the integrand of (3.33) to this proves the proposition. □

Similarly to the scattering cross-section $\sigma_{jk,nm}(\lambda)$ for the scattering system $\{H_0, H\}$, for $j, k \in \{l, r\}$ and $m, n \in \mathbb{N}_0$, we define

$$(\widehat{\sigma}_{ph}(\lambda))_{jk,nm} = \mathrm{Tr}((\widehat{T}_{ph}(\lambda))_{jk,nm}^*(\widehat{T}_{ph}(\lambda))_{jk,nm})$$

for the scattering system $\{H_{el}, H\}$, where

$$(\widehat{T}_{ph}(\lambda))_{jk,nm} = \widehat{P}_{j,n}(\lambda)\widehat{T}_{ph}(\lambda)\widehat{P}_{k,m}(\lambda)$$

with

$$\mathcal{M}(\widehat{P}_{j,n}(\lambda)) = \Phi_{H_{el}} W_+(H_{el}, H_0)P_{j,n}W_+^*(H_{el}, H_0)\Phi_{H_{el}}^*.$$

for a spectral representation $\Phi_{H_{el}}$ of H_{el}^{ac}. Note that Propositions 3.2.10 and 3.2.12 hold accordingly, i.e. for the two-level QD-LED given by (3.29), $(\widehat{\sigma}_{ph}(\lambda))_{jk,nm} = (\widehat{\sigma}_{ph}(\lambda))_{kj,mn}$ holds, and if $v_l = v_r$, we also have $(\widehat{\sigma}_{ph}(\lambda))_{jk,nm} = (\widehat{\sigma}_{ph}(\lambda))_{kj,nm}$.

Electron current

For $j \in \{l, r\}$ we may choose $-P_j = -p_j^{el} \otimes I_{ph}$ as observable Q. This is the observable of the number of electrons in the lead $\mathfrak{h}_j$, whose flux gives us the steady state electron current into this lead. The minus sign indicates the negative charge of the electrons. With this choice Assumption (A2) is obviously satisfied, and we can use the Landauer-Büttiker formula of Theorem 3.1.2 to calculate this current. Let us first consider the initial state ρ_0 as defined in (3.30). We obtain the Landauer-Büttiker formula in its well-known form.

Theorem 3.2.15. *For $j,k \in \{l,r\}$ with $j \neq k$, we have*

$$\mathfrak{J}_{j,\rho_0} = \mathfrak{J}_{-P_j,\rho_0} = -2\pi \int_{\mathbb{R}} \mathrm{d}\lambda (f_{FD}(\lambda-\mu_k) - f_{FD}(\lambda-\mu_j))\sigma_{jk}(\lambda).$$

Proof. Since $[P_j, H_j] = 0$ and $\rho_j = f_{FD}(H_j - \mu_j)$, $j \in \{l,S,r\}$, we get $[\rho_0, P_j] = 0$, whence the electron current $\mathfrak{J}_{j,\rho_0}$ is given by

$$\begin{aligned}\mathfrak{J}_{j,\rho_0} &= \frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{d}\lambda \,\mathrm{Tr}\Big(\rho_0(\lambda)(P_j(\lambda) - S^*(\lambda)P_j(\lambda)S(\lambda))\Big) \\ &= -2\pi \int_{\mathbb{R}} \mathrm{d}\lambda \,\mathrm{Tr}\Big(\rho_0(\lambda)(T^*(\lambda)P_j(\lambda)T(\lambda) - T^*(\lambda)T(\lambda)P_j(\lambda))\Big).\end{aligned} \tag{3.35}$$

Let $j,k \in \{l,r\}$ with $j \neq k$. Since $P_j(\lambda) + P_k(\lambda) = I_{\mathfrak{h}(\lambda)}$, we have

$$\begin{aligned}\mathfrak{J}_{j,\rho_0} &= -2\pi \int_{\mathbb{R}} \mathrm{d}\lambda \,\mathrm{Tr}\Big(\rho_0(\lambda)(T^*(\lambda)P_j(\lambda)T(\lambda) - T^*(\lambda)T(\lambda)P_j(\lambda))\Big) \\ &= -2\pi \int_{\mathbb{R}} \mathrm{d}\lambda \,\mathrm{Tr}\Big(\rho_0(\lambda)P_k(\lambda)T^*(\lambda)P_j(\lambda)T(\lambda) - T^*(\lambda)P_k(\lambda)T(\lambda)P_j(\lambda))\Big).\end{aligned} \tag{3.36}$$

The cyclicity of the trace gives

$$\mathfrak{J}_{j,\rho_0} = -2\pi \int_{\mathbb{R}} \mathrm{d}\lambda \,\Big(f_{FD}(\lambda-\mu_k)\mathrm{Tr}\big(T^*_{jk}(\lambda)T_{jk}(\lambda)\big) - f_{FD}(\lambda-\mu_j)\mathrm{Tr}\big(T^*_{kj}(\lambda)T_{kj}(\lambda)\big)\Big). \tag{3.37}$$

Since $\sigma_{jk}(\lambda) = \mathrm{Tr}\big(T^*_{jk}(\lambda)T_{jk}(\lambda)\big) = \sigma_{kj}(\lambda)$ by Lemma 3.2.7, we arrive at

$$\mathfrak{J}_{j,\rho_0} = -2\pi \int_{\mathbb{R}} \mathrm{d}\lambda \,(f_{FD}(\lambda-\mu_k) - f_{FD}(\lambda-\mu_j))\sigma_{jk}(\lambda). \tag{3.38}$$

□

We obtain all the usual consequences of the Landauer-Büttiker formula. In particular, the current flows from the lead with larger chemical potential into the lead with smaller chemical potential. The current vanishes for $\mu_l = \mu_r$. The initial state of the quantum dot has no impact on the final steady state current. Note that we obtain that the current into the left lead is the opposite of the current into the right lead, i.e. $\mathfrak{J}_{l,\rho_0} = -\mathfrak{J}_{r,\rho_0}$. This follows already from Corollary 3.1.3 and the fact that $\mathfrak{J}_{Q,\rho_0} = \mathfrak{J}_{-Q,\rho_0}$ since $P_l = P^{ac}_{H_0} - P_r$ gives us $\mathfrak{J}_{P_l,\rho_0} = \mathfrak{J}_{P^{ac}_{H_0}-P_r,\rho_0}$.

Let us now consider the case of $\widetilde{\rho}_0 = \widetilde{\rho}^{el}_0 \otimes \widetilde{\rho}^{ph}_0$. Since $h^{el} - h^{el}_0$ is trace class, we can apply the Landauer-Büttiker formula to calculate $\mathfrak{J}_{j,\widetilde{\rho}^{el}_0} = \mathfrak{J}_{-p^{el}_j,\widetilde{\rho}^{el}_0}$ as

$$\mathfrak{J}_{j,\widetilde{\rho}^{el}_0} = -2\pi \int_{\mathbb{R}} \mathrm{d}\lambda \,(f_{FD}(\lambda-\mu_k) - f_{FD}(\lambda-\mu_j))(\sigma_{el}(\lambda))_{jk},$$

where $j,k \in \{l,r\}$, $j \neq k$, and $(\sigma_{el}(\lambda))_{jk} = \mathrm{Tr}\big((t^{el}_{jk})^*(\lambda)t^{el}_{jk}(\lambda)\big)$ is the channel cross-section of the scattering system $\{h^{el}_0, h^{el}\}$ with transition matrix t^{el}.

Proposition 3.2.16. *For $j \in \{l, r\}$ the contact-induced current is equal to the current in the purely electric case, i.e.*

$$\mathfrak{J}^{el}_{j,\widetilde{\rho}_0} = \mathfrak{J}_{j,\widetilde{\rho}^{el}_0}.$$

Proof. Note that

$$e^{it(h^{el}\otimes I_{ph} + I_{el}\otimes h^{ph})} e^{-it(h^{el}_0\otimes I_{ph} + I_{el}\otimes h^{ph})} P^{ac}_{H_0} = e^{ith^{el}} e^{-ith^{el}_0} p^{ac}_{h^{el}_0} \otimes I_{ph},$$

whence $S_{el} = s_{el} \otimes I_{ph}$ and thus $S_{el}(\lambda) = \bigoplus_{n\in\mathbb{N}_0} s_{el}(\lambda - n\omega)$. We have

$$\begin{aligned}
\mathfrak{J}^{el}_{j,\widetilde{\rho}_0} &= \frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{d}\lambda\, \mathrm{Tr}\big(\widetilde{\rho}_0(\lambda)(P_j(\lambda) - S^*_{el}(\lambda)P_j(\lambda)S_{el}(\lambda))\big) \\
&= \frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{d}\lambda \sum_{n\in\mathbb{N}_0} (1 - e^{-\beta\omega}) e^{-\beta n\omega} \mathrm{Tr}\Big(\widetilde{\rho}^{el}_0(\lambda - n\omega)(p^{el}_j(\lambda - n\omega) \\
&\qquad\qquad - (s_{el})^*(\lambda - n\omega) p_j(\lambda - n\omega) s_{el}(\lambda - n\omega))\Big).
\end{aligned}$$

Note that the exponential decay in $\widetilde{\rho}^{ph} = (1 - e^{-\beta\omega})e^{-\beta h^{ph}}$ allows us to interchange the sum and the integral. It follows that

$$\begin{aligned}
\mathfrak{J}^{el}_{j,\widetilde{\rho}_0} &= \frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{d}\lambda\, \mathrm{Tr}\Big(\widetilde{\rho}_0(\lambda)\big(P_j(\lambda) - S^*_{el}(\lambda)P_j(\lambda)S_{el}(\lambda)\big)\Big) \\
&= \frac{1}{2\pi}\sum_{n\in\mathbb{N}_0} (1 - e^{-\beta\omega}) e^{-\beta n\omega} \int_{\mathbb{R}} \mathrm{d}\lambda\, \mathrm{Tr}\Big(\widetilde{\rho}^{el}_0(\lambda)(p^{el}_j(\lambda) - (s_{el})^*(\lambda) p_j(\lambda) s_{el}(\lambda))\Big) \qquad (3.39) \\
&= \frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{d}\lambda\, \mathrm{Tr}\Big(\widetilde{\rho}^{el}_0(\lambda)(p^{el}_j(\lambda) - (s_{el})^*(\lambda) p_j(\lambda) s_{el}(\lambda))\Big).
\end{aligned}$$

□

From this it is obvious that the contact-induced current vanishes if the chemical potentials of the electrons in both leads are equal. However, the photon-induced current does not have to be zero since $\widetilde{\rho}_0$ is a steady state, but not an equilibrium state. In fact, choosing $\mu = \mu_l = \mu_r$ and $\widetilde{\rho}^{el}_0 = f_{FD}(h^{el}_0 - \mu)$ implies

$$\widetilde{\rho}_{el} = w^{el}_-(h^{el}, h^{el}_0)\widetilde{\rho}^{el}_0 (w^{el}_-(h^{el}, h^{el}_0))^* \otimes \widetilde{\rho}^{ph}_0 = f_{FD}\big((h^{el})^{ac} - \mu\big) \otimes \widetilde{\rho}^{ph}_0,$$

and this gives us the following proposition.

Proposition 3.2.17. *For $\widetilde{\rho}^{el}_0 = f_{FD}(h^{el}_0 - \mu)$, we have*

$$\begin{aligned}
\mathfrak{J}^{ph}_{j,\widetilde{\rho}_0} = \frac{1 - e^{-\beta\omega}}{2\pi}\int_{\mathbb{R}} \mathrm{d}\lambda \sum_{k\in\{l,r\}} \sum_{n,m\in\mathbb{N}_0} &(\widehat{\sigma}_{ph}(\lambda))_{jk,mn} \\
&\times \big(f_{FD}(\lambda - \mu - m\omega)e^{-\beta m\omega} - f_{FD}(\lambda - \mu - n\omega)e^{-\beta n\omega}\big).
\end{aligned}$$

Proof. Setting $P_{j,el} = W_+(H_{el}, H_0)P_jW_+^*(H_{el}, H_0)$, we have

$$\begin{aligned}\mathfrak{J}_{j,\widetilde{\rho}_0}^{ph} &= \frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{d}\lambda\, \mathrm{Tr}(\widehat{\widetilde{\rho}_{el}}(\lambda)(\widehat{P}_{j,el}(\lambda) - \widehat{S}_{ph}^*(\lambda)\widehat{P}_{j,el}(\lambda)\widehat{S}_{ph}(\lambda))) \\ &= \frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{d}\lambda \sum_{k\in\{l,r\}}\sum_{n,m\in\mathbb{N}_0} f_{FD}(\lambda-\mu-n\omega)(1-e^{-\beta\omega})e^{-\beta n\omega} \\ &\qquad\qquad \times \mathrm{Tr}\Big(\delta_{jk}\delta_{nm} - (\widehat{S}_{ph}(\lambda))^*_{jk,mn}(\widehat{S}_{ph}(\lambda))_{jk,mn}\Big).\end{aligned}$$

Since S_{ph} is unitary, we can use

$$I_{\mathfrak{h}_n(\lambda)} - (\widehat{S}_{ph}(\lambda))^*_{nn}(\widehat{S}_{ph}(\lambda))_{nn} = \sum_{\substack{m\in\mathbb{N}_0\\ m\neq n}} (\widehat{S}_{ph}(\lambda))^*_{mn}(\widehat{S}_{ph}(\lambda))_{mn}$$

to obtain

$$\begin{aligned}\mathfrak{J}_{j,\widetilde{\rho}_0}^{ph} &= \frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{d}\lambda \sum_{k\in\{l,r\}}\sum_{n,m\in\mathbb{N}_0} f_{FD}(\lambda-\mu-n\omega)(1-e^{-\beta\omega})e^{-\beta n\omega} \\ &\qquad\qquad \times \mathrm{Tr}\Big((\widehat{S}_{ph}(\lambda))^*_{kj,mn}(\widehat{S}_{ph}(\lambda))_{kj,mn} - (\widehat{S}_{ph}(\lambda))^*_{jk,mn}(\widehat{S}_{ph}(\lambda))_{jk,mn}\Big) \\ &= \frac{1-e^{-\beta\omega}}{2\pi}\int_{\mathbb{R}} \mathrm{d}\lambda \sum_{k\in\{l,r\}}\sum_{n,m\in\mathbb{N}_0} \big(\widehat{\sigma}_{ph}(\lambda)\big)_{jk,mn} \\ &\qquad\qquad \times \Big(f_{FD}(\lambda-\mu-m\omega)e^{-\beta m\omega} - f_{FD}(\lambda-\mu-n\omega)e^{-\beta n\omega}\Big).\end{aligned}$$

□

Depending on the choice of the parameters of the QD-LED, e.g. the potentials v_l and v_r, or the eigenvectors e_m, $1 \le m \le d$, Proposition 3.2.17 allows for a photon-induced current of either sign or even zero. In the case of the two-level QD-LED given by (3.29), the photon-induced current and hence the total current is in fact zero.

Corollary 3.2.18. *Let $\{H_0, H\}$ be the two-level QD-LED given by* (3.29) *and $v_l = v_r$. Furthermore, let $\widetilde{\rho}_0^{el} = f_{FD}(h_0^{el} - \mu)$. Then $\mathfrak{J}_{j,\widetilde{\rho}_0} = 0$ for $j \in \{l, r\}$.*

Proof. Let $j, k \in \{l, r\}$ and $n, m \in \mathbb{N}_0$. Proposition 3.2.14 gives us $\mathfrak{J}_{j,\widetilde{\rho}_0} = \mathfrak{J}^{el}_{j,\widetilde{\rho}_0} + \mathfrak{J}^{ph}_{j,\widetilde{\rho}_0}$. By Proposition 3.2.16, we have $\mathfrak{J}^{el}_{j,\widetilde{\rho}_0} = 0$. Also,

$$\big(\widehat{\sigma}_{ph}(\lambda)\big)_{jk,nm} = \big(\widehat{\sigma}_{ph}(\lambda)\big)_{kj,mn} = \big(\widehat{\sigma}_{ph}(\lambda)\big)_{jk,mn}$$

for a.e. $\lambda \in \mathbb{R}$ by the analog of Propositions 3.2.10 and 3.2.12 for $\widehat{\sigma}_{ph}$. Thus, we obtain

$$\begin{aligned}\mathfrak{J}_{j,\widetilde{\rho}_0}^{ph} &= \frac{1-e^{-\beta\omega}}{2\pi}\int_{\mathbb{R}} \mathrm{d}\lambda \sum_{k\in\{l,r\}}\sum_{n,m\in\mathbb{N}_0} f_{FD}(\lambda-n\omega)e^{-\beta n\omega} \\ &\qquad\qquad \times \big((\widehat{\sigma}_{ph}(\lambda))_{jk,nm} - (\widehat{\sigma}_{ph}(\lambda))_{jk,mn}\big) \\ &= 0,\end{aligned}$$

which proves the corollary. □

In the next section we will see that although the electron current is zero, the photon production rate is non-zero for the two-level quantum dot with initial state $\widetilde{\rho}_0$.

Photon production rate

Let

$$\mathfrak{N} = I_{el} \otimes \mathfrak{N}_+,$$

where $\mathfrak{N}_+ = \mathrm{d}\Gamma(I_{ph}) = a^*a$ is the photon number operator on $\mathfrak{h}^{ph} = \mathfrak{F}_+(\mathbb{C})$, which is self-adjoint and commutes with h^{ph}. It follows that $\mathfrak{N}$ is also self-adjoint and commutes with H_0. It is not bounded, but since $\mathrm{dom}(\mathfrak{N}_+) = \mathrm{dom}(h^{ph})$, it is immediately obvious that $\mathfrak{N}(H_0 + \theta)^{-1}$ is bounded, whence $\mathfrak{N}$ satisfies Assumption (A2) and is admissible as Q in the Landauer-Büttiker formula. $\mathfrak{N}$ allows us to calculate the photon production rate in the steady state. For the calculations in this section, note the fact that

$$(\mathfrak{N}(\lambda))_{jk,nm} = n\, P_{j,n}(\lambda) P_{k,m}(\lambda), \qquad j,k \in \{l,r\}, \qquad n,m \in \mathbb{N}_0.$$

Recall that the contact-induced flux is the flux that is induced by the coupling of the leads only, not taking into account the electron-photon interaction. It is physically obvious that the contact-induced photon production rate should be zero. The following proposition confirms this.

Proposition 3.2.19. *We have* $\mathfrak{J}^{el}_{\mathfrak{N},\widetilde{\rho}_0} = \mathfrak{J}^{el}_{\mathfrak{N},\rho_0} = 0$.

Proof. We have $(S_{el}(\lambda))_{nm} = s_{el}(\lambda - n\omega)\delta_{nm}$. Just as in (3.39), we have

$$\mathfrak{J}^{el}_{\mathfrak{N},\widetilde{\rho}_0} = -\frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{d}\lambda \sum_{n\in\mathbb{N}_0} \widetilde{\rho}_0^{ph}(n)\mathrm{Tr}\Big(\widetilde{\rho}_0^{el}(\lambda)(n - n(s_{el})^*(\lambda)s_{el}(\lambda))\Big) = 0, \tag{3.40}$$

where we used the unitarity of $s_{el}(\lambda)$. Similarly,

$$\mathfrak{J}^{el}_{\mathfrak{N},\rho_0} = -\frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{d}\lambda\, \rho_0(\lambda) \sum_{n\in\mathbb{N}_0} \mathrm{Tr}\Big(n - n(s_{el})^*(\lambda)s_{el}(\lambda)\Big) = 0. \tag{3.41}$$

□

Again, we start with the initial state ρ_0. The Landauer-Büttiker formula gives us a formula for the photon production rate.

Proposition 3.2.20. *The photon production rate for the initial state* ρ_0 *satisfies*

$$\mathfrak{J}_{\mathfrak{N},\rho_0} = -2\pi\int_{\mathbb{R}} \mathrm{d}\lambda \sum_{j,k\in\{l,r\}} \sum_{m,n\in\mathbb{N}_0} f_{FD}(\lambda - \mu_k)(n-m)\sigma_{jk,mn}(\lambda).$$

Proof. Note that $P_j(\lambda)\mathfrak{N}(\lambda) = \mathfrak{N}(\lambda)P_j(\lambda)$ for $j \in \{l, r\}$, whence

$$\begin{aligned}\mathfrak{J}_{\mathfrak{N},\rho_0} &= -2\pi \int_{\mathbb{R}} \mathrm{d}\lambda \,\mathrm{Tr}\Big(\rho_0(\lambda)\big(T^*(\lambda)T(\lambda)\mathfrak{N}(\lambda) - T^*(\lambda)\mathfrak{N}(\lambda)T(\lambda)\big)\Big) \\ &= -2\pi \int_{\mathbb{R}} \mathrm{d}\lambda \sum_{j,k\in\{l,r\}} \sum_{m,n\in\mathbb{N}_0} f_{FD}(\lambda-\mu_k) \\ &\qquad\qquad \times \mathrm{Tr}\big(n\,T^*_{jk,mn}(\lambda)T_{jk,mn}(\lambda) - m\,T^*_{jk,mn}(\lambda)T_{jk,mn}(\lambda)\big) \\ &= -2\pi \int_{\mathbb{R}} \mathrm{d}\lambda \sum_{j,k\in\{l,r\}} \sum_{m,n\in\mathbb{N}_0} f_{FD}(\lambda-\mu_k)(n-m)\sigma_{jk,mn}(\lambda).\end{aligned}$$

□

Consider now the case $\widetilde{\rho}_0$. With the same calculations as in the proof above we obtain the following formula for the photon production rate.

Proposition 3.2.21. *The photon production rate for the initial state $\widetilde{\rho}_0$ satisfies*

$$\mathfrak{J}_{\mathfrak{N},\widetilde{\rho}_0} = -2\pi \int_{\mathbb{R}} \mathrm{d}\lambda \sum_{j,k\in\{l,r\}} \sum_{m,n\in\mathbb{N}_0} \widetilde{\rho}_0(\lambda,k,n)(n-m)\sigma_{jk,mn}(\lambda),$$

where $\widetilde{\rho}_0(\lambda,n,k) = f_{FD}(\lambda - n\omega - \mu_k)(1-e^{-\beta\omega})e^{-\beta n\omega}$.

Let us get back to the two-level QD-LED. Recall that in the case of $\mu_l = \mu_r$ the electron current is zero. However, the photon production rate is positive.

Proposition 3.2.22. *For the two-level QD-LED given by* (3.29) *and $v_l = v_r$, it holds that $\mathfrak{J}_{\mathfrak{N},\widetilde{\rho}_0} > 0$ if $\mu = \mu_l = \mu_r$.*

Proof. Let $\widetilde{\rho}_0(\lambda,n) = (1+e^{\beta(\lambda-n\omega-\mu)})^{-1}(1-e^{-\beta\omega})e^{-\beta n\omega}$. Since $\sigma_{jk,mn}(\lambda) = \sigma_{jk,nm}(\lambda)$, we have

$$\begin{aligned}\mathfrak{J}_{\mathfrak{N},\widetilde{\rho}_0} &= -2\pi \int_{\mathbb{R}} \mathrm{d}\lambda \,\mathrm{Tr}(\widetilde{\rho}_0(\lambda)(T^*(\lambda)T(\lambda)\mathfrak{N}(\lambda) - T^*(\lambda)\mathfrak{N}(\lambda)T(\lambda))) \\ &= -2\pi \int_{\mathbb{R}} \mathrm{d}\lambda \sum_{n,m\in\mathbb{N}_0} \sum_{j,k\in\{l,r\}} \widetilde{\rho}_0(\lambda,m)(m-n)\sigma_{jk,nm}(\lambda) \\ &= -2\pi \int_{\mathbb{R}} \mathrm{d}\lambda \sum_{\substack{n,m\in\mathbb{N}_0 \\ n>m}} \sum_{j,k\in\{l,r\}} (n-m)(\widetilde{\rho}_0(\lambda,n) - \widetilde{\rho}_0(\lambda,m))\sigma_{jk,nm}(\lambda).\end{aligned}$$

But $\rho_0(\lambda,n)$ is monotonously decreasing, which gives us $\mathfrak{J}_{\mathfrak{N},\widetilde{\rho}_0} > 0$ since the scattering system $\{H_{el}, H\}$ is non-trivial. □

The positive photon production rate in Proposition 3.2.22 is in fact plausible. Since $\widetilde{\rho}_0$ with $\mu_l = \mu_r$ is a steady state, but not an equilibrium state, it is not to be expected that all fluxes vanish. This photon production is actually a consequence of our modeling approach. Recall that we have infinitely many electrons that may relax into a lower energy state by emitting a photon or get excited by absorbing a photon. Depending on the availability of high-energy electrons and absorbable photons, these processes might

not cancel out. In the case of Proposition 3.2.22, there is an excess of electrons relaxing into lower energy states by emitting photons. However, since the setup is completely mirror symmetric, the electrons will travel from left to right and from right to left with equal probability. Hence, no net current is produced. We already referred to this effect in the introduction. In a real physical system, the electrons can not relax into a lower energy state since all those states are occupied and, being fermions, no two electrons may occupy the same state. But in our model the electrons are labeled by the number of photons in their photon field, whence (λ^{el}, n) and (λ^{el}, m) can be occupied simultaneously for any electron energy $\lambda^{el} \in \mathbb{R}$ and photon numbers $n, m \in \mathbb{N}_0$, $n \neq m$. Note that the energy of the systems is conserved, whence the total energy of the electrons has to decrease with the same rate as the photon energy increases. Indeed, choose the observable $h_0^{el} \otimes I_{ph}$ to obtain

$$\begin{aligned}
\mathfrak{J}_{h_0^{el},\widetilde{\rho}_0} &= -2\pi \int_{\mathbb{R}} \mathrm{d}\lambda \sum_{m,n\in\mathbb{N}_0} \sum_{j,k\in\{l,r\}} \widetilde{\rho}_0(\lambda, m)\big((\lambda - m\omega) - (\lambda - n\omega)\big)\sigma_{jk,nm}(\lambda) \\
&= -2\pi \int_{\mathbb{R}} \mathrm{d}\lambda \sum_{\substack{n,m\in\mathbb{N}_0 \\ m<n}} \sum_{j,k\in\{l,r\}} \omega(m-n)(\widetilde{\rho}_0(\lambda, n) - \widetilde{\rho}_0(\lambda, m))\sigma_{jk,nm}(\lambda) \\
&= -\omega\, \mathfrak{J}_{\mathfrak{N},\widetilde{\rho}_0}.
\end{aligned}$$

In all the above formulae, the remaining unknown object is the scattering cross-section. Since the perturbation in the scattering system $\{H_0, H\}$ of the Jaynes-Cummings QD-LED is not a finite rank perturbation, the calculation of scattering cross-section, or alternatively of the transition matrix, is far from trivial. In the next chapter we address this topic and prove a formula for the transition matrix that is even more explicit than Proposition 3.1.6.

4 Boundary triplets and the scattering matrix of the Jaynes-Cummings quantum dot LED

In the previous Chapter 3 we proved an abstract Landauer-Büttiker formula and applied it to a model of a QD-LED based on the Jaynes-Cummings model. As a result, we obtained formulae that express the steady state electric current and the steady state photon production rate in terms of the channel cross-sections $\sigma_{jk,nm}(\lambda)$. To actually calculate these quantities, we need to know the scattering matrix of the system. However, Proposition 3.1.6 gives us the transition matrix only in terms of the resolvent of H, which is an object about which we do not know much. The goal of this chapter is to give a formula for the scattering matrix in terms of more tractable objects. The main tool for this is the concept of boundary triplets and their Weyl functions, which allow us to describe H by an extension operator B. We then use the fact that B^{-1} is trace class to construct a spectral representation of H_0 similar to the one we used in Proposition 3.1.6. But the special choice of the representation leads to a much more explicit formula than before. This formula is the generalization of the result for finite rank couplings that was proven by Behrndt et al. [12].

In Section 4.1 we provide the necessary background information on boundary triplets that we need to formulate and prove the representation of the scattering matrix in Theorem 4.1.14. In Section 4.2 we construct a boundary triplet for the Jaynes-Cummings QD-LED of Section 3.2 and apply the new representation of the scattering matrix. We show that the formula for the scattering matrix that we obtain is indeed very useful, and we calculate the transition matrix explicitly for a special case of the Jaynes-Cummings QD-LED.

4.1 Boundary triplets and the scattering matrix

Let A be a closed symmetric operator on some Hilbert space $\mathfrak{H}$. If A is densely defined, any symmetric extension $\widetilde{A} \supset A$ satisfies $\widetilde{A} \subset \widetilde{A}^* \subset A^*$, whence symmetric extensions of A can be described as restrictions of A^*. Boundary triplets can be used to describe all closed extensions of a given closed symmetric operator A. If A is not densely defined, then the operator A^* does not exist. However, a corresponding object can be defined in the language of linear relations. This is important for us since in Section 4.2.2 we choose a non-densely defined operator A in the treatment of the QD-LED based on the Jaynes-Cummings model that we introduced in Section 3.2.

4.1.1 Linear relations

Let $\mathfrak{H}$ be a Hilbert space. Any operator $A \in \mathfrak{L}(\mathfrak{H})$ is completely described by its graph

$$\Theta_A = \{(f, f') \in \mathfrak{H}^2 \,|\, f \in \mathrm{dom}(A), f' = Af\} \subset \mathfrak{H} \oplus \mathfrak{H},$$

which is a subspace of $\mathfrak{H} \oplus \mathfrak{H}$. If a particular subspace of $\mathfrak{H} \oplus \mathfrak{H}$ is not the graph of a linear operator, the notion of linear relations becomes useful (cf. [12] and references therein).

Definition 4.1.1. *Let $\mathfrak{H}$ be a Hilbert space. A* (closed) linear relation Θ *on $\mathfrak{H}$ is a (closed) subspace of $\mathfrak{H} \oplus \mathfrak{H}$. We denote the set of all closed linear relations by $\widetilde{\mathfrak{C}}(\mathfrak{H})$. Furthermore,*

$$\begin{aligned} \mathrm{dom}(\Theta) &= \{f \in \mathfrak{H} \,|\, \exists\, f' \in \mathfrak{H} : (f, f') \in \Theta\}, & \ker(\Theta) &= \{f \in \mathfrak{H} \,|\, (f, 0) \in \Theta\} \\ \mathrm{ran}(\Theta) &= \{f' \in \mathfrak{H} \,|\, \exists\, f \in \mathfrak{H} : (f, f') \in \Theta\}, & \mathrm{mul}(\Theta) &= \{f' \in \mathfrak{H} \,|\, (0, f') \in \Theta\} \end{aligned}$$

denote the domain, kernel, range, *and the* multi-valued part *of Θ, respectively. The adjoint relation is given by*

$$\Theta^* = \{(f, f') \in \mathfrak{H}^2 \,|\, \forall\, (g, g') \in \Theta \,:\, (g, f') = (g', f)\}.$$

The linear relation Θ is called symmetric *if $\Theta \subset \Theta^*$. It is called* self-adjoint *if $\Theta = \Theta^*$. For two linear relations $\Theta_1, \Theta_2 \subset \mathfrak{H}^2$, we have the operations*

$$\begin{aligned} \Theta_1 + \Theta_2 &= \{(f, f_1' + f_2') \,|\, (f, f_1') \in \Theta_1, (f, f_2') \in \Theta_2\}, \\ \Theta_1\Theta_2 &= \{(f, f_1') \,|\, \exists\, f_2' \in \mathfrak{H} \,:\, (f, f_2') \in \Theta_2, (f_2', f_1') \in \Theta_1\}, \\ \Theta_1^{-1} &= \{(f', f) \,|\, (f, f') \in \Theta_1\}, \\ \Theta_1 \oplus \Theta_2 &= \{(f_1 \oplus f_2, f_1' \oplus f_2') \subset \mathfrak{H}^2 \oplus \mathfrak{H}^2 \,|\, (f_j, f_j') \in \Theta_j, j \in \{1, 2\}\}. \end{aligned}$$

If $A, \widetilde{A} \in \mathfrak{L}(\mathfrak{H})$ are linear operators, we denote their graphs by Θ_A and $\Theta_{\widetilde{A}}$, respectively. We can apply all the notions introduced in the previous definition to Θ_A and $\Theta_{\widetilde{A}}$. They coincide with the respective objects for the linear operators A and $\widetilde{A}$, i.e. $\mathrm{dom}(\Theta_A) = \mathrm{dom}(A)$, $\Theta_A + \Theta_{\widetilde{A}} = \Theta_{A+\widetilde{A}}$, and so forth. This is why we identify operators $A \in \mathfrak{L}(\mathfrak{H})$ with their graphs Θ_A from now on. In this sense, we define the set $\mathfrak{C}(\mathfrak{H}) \subset \widetilde{\mathfrak{C}}(\mathfrak{H})$ of all closed linear operators on $\mathfrak{H}$. The multi-valued part of Θ_A is zero. In fact, any relation $\Theta \subset \mathfrak{H}^2$ is the graph of an operator if and only if $\mathrm{mul}(\Theta) = \{(0, 0)\}$. We have $\mathrm{mul}(A^*) = (\mathrm{dom}(A))^\perp$, whence A^* is an operator if and only if A is densely defined. We also have the relation $\ker(A^*) = \mathrm{ran}(A)^\perp$. In the following we use the notation $\vec{f} = (f, f')$ for the elements $\vec{f} \in \Theta$ of a linear relation. We can also define the resolvent and the spectrum of a closed linear relation.

Definition 4.1.2. *Let Θ be a closed linear relation on the Hilbert space $\mathfrak{H}$. Then the* resolvent set $\rho(\Theta) \subset \mathbb{C}$ *is the set of all complex numbers $\zeta \in \mathbb{C}$ such that $(\Theta - \zeta)^{-1}$ is an everywhere defined bounded operator on $\mathfrak{H}$. Furthermore, $\sigma(\Theta) = \mathbb{C} \setminus \rho(\Theta)$ defines the* spectrum *of Θ.*

4.1.2 Boundary triplets and their properties

We can now introduce the notion of a boundary triplet, which allows us to describe all extensions of $A \in \mathfrak{L}(\mathfrak{H})$ using an extension parameter $\Theta \in \widetilde{\mathfrak{C}}(\mathcal{H})$. This leads to the Krein-type resolvent formula, cf. Lemma 4.1.8, which is important for the formula of the scattering matrix. For detailed information on boundary triplets, in particular for proofs of the statements in this section, see [12, 63] and references therein.

Definition 4.1.3. *Let $\mathfrak{H}$ be a Hilbert space and $A \in \mathfrak{L}(\mathfrak{H})$ a closed symmetric operator. Then a* boundary triplet $\Pi = (\mathcal{H}, \Gamma_0, \Gamma_1)$ *for A^* consists of a Hilbert space $\mathcal{H}$ and two linear operators $\Gamma_j : A^* \to \mathcal{H}$, $j \in \{0, 1\}$, such that*

$$\Gamma = (\Gamma_0, \Gamma_1) : A^* \to \mathcal{H} \oplus \mathcal{H}$$

is surjective and Green's identity

$$\langle f', g\rangle - \langle f, g'\rangle = \langle \Gamma_1 \vec{f}, \Gamma_0 \vec{g}\rangle - \langle \Gamma_0 \vec{f}, \Gamma_1 \vec{g}\rangle, \qquad \vec{f} = (f, f'), \vec{g} = (g, g') \in \mathfrak{H}^2,$$

holds.

Remark 4.1.4. *For any closed symmetric operator $A \in \mathfrak{L}(\mathfrak{H})$, a boundary triplet for A^* always exists. However, it is not at all unique. In the case of a densely defined operator A, one usually defines Γ on $\mathrm{dom}(A^*) \subset \mathfrak{H}$ and equips this with the graph norm. Note that this coincides with the usual $\mathfrak{H}^2$-norm on $A^* \subset \mathfrak{H}^2$ since $\vec{f} \in A^*$ implies $\vec{f} = (f, A^* f)$ and $\|\vec{f}\|^2_{\mathfrak{H}^2} = \|f\|^2_{\mathfrak{H}} + \|A^* f\|^2_{\mathfrak{H}}$ if A^* is an operator.*

We have the following properties of a boundary triplet.

Proposition 4.1.5. *Let $A \in \mathfrak{L}(\mathfrak{H})$ be closed and symmetric and let $\Pi = (\mathcal{H}, \Gamma_0, \Gamma_1)$ be a boundary triplet for A^*. Then the mapping*

$$\widetilde{\mathfrak{C}}(\mathcal{H}) \ni \Theta \mapsto A_\Theta = \{\vec{f} \in A^* \,|\, (\Gamma_0 \vec{f}, \Gamma_1 \vec{f}) \in \Theta\} \in \mathfrak{C}(\mathfrak{H}) \tag{4.1}$$

is a bijection between the closed linear relations on $\mathfrak{H}$ and the closed extensions of A. The relation Θ is called the extension parameter. *Moreover, A_Θ is self-adjoint if and only if Θ is self-adjoint.*

Note that we can rewrite relation (4.1) as $A_\Theta = \ker(\Gamma_1 - \Theta\Gamma_0)$ using sum, product, and kernel in the sense of linear relations as introduced in Definition 4.1.1. There are the two special extensions $A_0 = \ker(\Gamma_0)$ corresponding to the *pure relation*

$$\Theta_\infty = \{(0, f') \,|\, f' \in \mathfrak{H}\}$$

and $A_1 = \ker(\Gamma_1)$ corresponding to the null operator $\Theta_0 = \{(f, 0) \,|\, f \in \mathfrak{H}\}$. Note that Θ_0 and Θ_∞ are self-adjoint, whence A_0 and A_1 are also self-adjoint. For $\zeta \in \rho(A_0)$, define $\mathcal{N}_\zeta = \ker(A^* - \zeta)$ and

$$\vec{\mathcal{N}}_\zeta = \{(f, \zeta f) \in \mathfrak{H}^2 \,|\, f \in \mathcal{N}_\zeta\} \subset \mathfrak{H} \oplus \mathfrak{H}.$$

With $\vec{\mathcal{N}}_\zeta$ we can define two very important objects in the theory of boundary triplets, the γ-field and the Weyl function. They are operator-valued functions defined on the

resolvent set of A_0 and are strongly connected to the spectral properties of the extensions A_Θ, $\Theta \in \widetilde{\mathfrak{C}}(\mathfrak{H})$.

Definition 4.1.6. *Let A be a closed symmetric operator and let $\Pi = (\mathcal{H}, \Gamma_0, \Gamma_1)$ be a boundary triplet for A^*. Let $P^1_{\mathfrak{H}}$ denote the orthogonal projection onto the first component of $\mathfrak{H}^2$. Then the* γ-field *is defined as*

$$\gamma : \rho(A_0) \to \mathfrak{B}(\mathcal{H}, \mathfrak{H}), \qquad \gamma(\zeta) = P^1_{\mathfrak{H}}(\Gamma_0 \restriction \vec{\mathcal{N}}_\zeta)^{-1}. \tag{4.2}$$

The Weyl function *is defined as*

$$M : \rho(A_0) \to \mathfrak{B}(\mathcal{H}), \qquad M(\zeta) = \Gamma_1(\Gamma_0 \restriction \vec{\mathcal{N}}_\zeta)^{-1}. \tag{4.3}$$

The γ-field and the Weyl function are indeed well-defined, which is due to the fact that $A^* = \ker(\Gamma_0) \oplus \vec{\mathcal{N}}_\zeta$ for $\zeta \in \rho(A_0)$.

Lemma 4.1.7. *The γ-field given by* (4.2) *and the Weyl function given by* (4.3) *of a boundary triplet are well-defined holomorphic functions. Furthermore, the inverse $\gamma(\zeta)^{-1} \in \mathfrak{B}(\mathfrak{H}, \mathcal{H})$ exists for every $\zeta \in \rho(A_0)$ and*

$$\gamma(\zeta_2) = \big(1 + (\zeta_2 - \zeta)(A_0 - \zeta_2)^{-1}\big)\gamma(\zeta)$$

as well as

$$M(\zeta) - M(\zeta_2)^* = (\zeta - \overline{\zeta_2})\gamma(\zeta_2)^*\gamma(\zeta). \tag{4.4}$$

for every $\zeta, \zeta_2 \in \rho(A_0)$.

If we choose $\zeta_2 = \overline{\zeta}$ in (4.4), we see that $M(\overline{\zeta}) = M(\zeta)^*$. With $\zeta_2 = \zeta$ we obtain that $\Im\mathrm{m}(M(\zeta)) = \Im\mathrm{m}(\zeta)\gamma(\zeta)^*\gamma(\zeta) \geq 0$ for $\zeta \in \mathbb{C}_+$. A holomorphic function with these properties is called *Nevanlinna function*. Since $\gamma(\zeta)$ is invertible, we also get that $M(\zeta)$ is invertible for $\Im\mathrm{m}(\zeta) \neq 0$. The γ-field and the Weyl function can be used to express the resolvent of an extension A_Θ, $\Theta \in \widetilde{\mathfrak{C}}(\mathfrak{H})$, in terms of the extension parameter Θ and the resolvent of the extension A_0. This representation is the basis of our formula of the scattering matrix in terms of the Weyl function. It is called a *Krein-type resolvent formula* [12].

Lemma 4.1.8. *Let A be a closed symmetric operator and let $\Pi = (\mathcal{H}, \Gamma_0, \Gamma_1)$ be a boundary triplet for A^*. Let $A_0 = \ker(\Gamma_0)$ and let $\Theta \in \widetilde{\mathfrak{C}}(\mathfrak{H})$. Then*

$$(A_\Theta - \zeta)^{-1} = (A_0 - \zeta)^{-1} - \gamma(\zeta)\big(\Theta - M(\zeta)\big)^{-1}\gamma(\overline{\zeta})^*, \qquad \zeta \in \rho(A_0) \cap \rho(A_\Theta).$$

4.1.3 Direct sums of boundary triplets

In Section 4.2.2 we use the spectral decomposition $H_0 = \bigoplus_{n\in\mathbb{N}_0} H_0^{(n)}$ and construct boundary triplets for the summands $H_0^{(n)}$. We want to be able to obtain a boundary triplet for H_0 as a direct sum of the boundary triplets for $H_0^{(n)}$. For two boundary triplets $\Pi^{(j)} = (\mathcal{H}^{(j)}, \Gamma_0^{(j)}, \Gamma_1^{(j)})$, $j \in \{1, 2\}$, the direct sum $\Pi = \Pi^{(1)} \oplus \Pi^{(2)}$ is again a boundary triplet $\Pi = (\mathcal{H}, \Gamma_0, \Gamma_1)$ defined by

$$\mathcal{H} = \mathcal{H}^{(1)} \oplus \mathcal{H}^{(2)}, \qquad \Gamma_0 = \Gamma_0^{(1)} \oplus \Gamma_0^{(2)}, \qquad \Gamma_1 = \Gamma_1^{(1)} \oplus \Gamma_1^{(2)}.$$

It is easy to see that this is indeed a boundary triplet. Green's identity holds in both components, whence it holds for the direct sum as well. The same is true for the surjectivity. By induction we can define the direct sum of any finite number of boundary triplets. However, if we take a family $\{\Pi^{(n)}\}_{n\in\mathbb{N}}$, the direct sum is in general not a boundary triplet since Γ might be ill-defined as an operator on A^* or it might not be surjective. In this section we prove that we do obtain a boundary triplet if the Weyl function $M^{(n)}$ of every summand satisfies $M^{(n)}(i) = i$, $n \in \mathbb{N}$. The following lemma shows that we can transform any boundary triplet such that this condition holds. It appeared in [62] for the case of a densely defined closed symmetric operator A. We formulate it for the more general case of an arbitrary closed symmetric operator. The proof is essentially identical and differs only in formalities. This also applies to Lemma 4.1.10 and Theorem 4.1.11. Note that in the remainder of this chapter we use the letter Q to denote the real part of the Weyl function. We choose this notation to conform to the notation in [12]. No confusion with the usage of Q as an observable is possible since Q does not appear with this meaning in this chapter.

Lemma 4.1.9. *Let A be a closed symmetric operator on a Hilbert space $\mathfrak{H}$ and let $\widetilde{\Pi} = (\mathcal{H}, \widetilde{\Gamma}_0, \widetilde{\Gamma}_1)$ be a boundary triplet for A^*. Furthermore, let $\widetilde{M}(i) = Q + iR^2$ with*

$$Q = \Re\mathrm{e}(M(i)), \qquad R = \sqrt{\Im\mathrm{m}(M(i))}.$$

Then $(\mathcal{H}, \Gamma_0, \Gamma_1)$ given by

$$\Gamma_0 = R\widetilde{\Gamma}_0 \qquad \textit{and} \qquad \Gamma_1 = R^{-1}(\widetilde{\Gamma}_1 - Q\widetilde{\Gamma}_0)$$

is a boundary triplet for A^* with Weyl function M satisfying $\ker(\Gamma_0) = \ker(\widetilde{\Gamma}_0)$ and $M(i) = i$.

Proof. If $\widetilde{\gamma}$ is the γ-field of $\widetilde{\Pi}$, the Weyl function always satisfies

$$\Im\mathrm{m}(\widetilde{M}(\zeta)) \geq \Im\mathrm{m}(\zeta)\widetilde{\gamma}(\zeta)^*\widetilde{\gamma}(\zeta).$$

Since $\widetilde{\gamma}$ is invertible, R^{-1} is a well-defined bounded self-adjoint operator. For every $\vec{f} = (f, f') \in A^*$ and $\vec{g} = (g, g') \in A^*$,

$$\langle \Gamma_0\vec{f}, \Gamma_1\vec{g}\rangle = \langle \widetilde{\Gamma}_0\vec{f}, \widetilde{\Gamma}_1\vec{g}\rangle - \langle \widetilde{\Gamma}_0\vec{f}, Q\widetilde{\Gamma}_0\vec{g}\rangle.$$

Using $Q = Q^*$, we see that

$$\langle \Gamma_0\vec{f}, \Gamma_1\vec{g}\rangle - \langle \Gamma_1\vec{f}, \Gamma_0\vec{g}\rangle = \langle \widetilde{\Gamma}_0\vec{f}, \widetilde{\Gamma}_1\vec{g}\rangle - \langle \widetilde{\Gamma}_1\vec{f}, \widetilde{\Gamma}_0\vec{g}\rangle,$$

whence Green's identity holds. Let $(v, w) \in \mathcal{H} \oplus \mathcal{H}$. Since $\widetilde{\Gamma}$ is surjective, we can choose $\vec{f}$ such that

$$\widetilde{\Gamma}_0\vec{f} = R^{-1}v, \qquad \widetilde{\Gamma}_1\vec{f} = Rw + QR^{-1}v.$$

We obtain $\Gamma_0\vec{f} = v$ and

$$\Gamma_1\vec{f} = R^{-1}(Rw + QR^{-1}v - QR^{-1}v) = w.$$

Thus, Γ is also surjective and Π is indeed a boundary triplet for A^*. Obviously, we have $\ker(\Gamma_0) = \ker(\widetilde{\Gamma}_0)$. For $\zeta \in \mathbb{C} \setminus \mathbb{R}$ and $\vec{f}_\zeta \in \vec{\mathcal{N}}_\zeta$,

$$\Gamma_1 \vec{f}_\zeta = R^{-1}(\widetilde{M}(\zeta) - Q)R^{-1}\Gamma_0,$$

whence $M(\zeta) = R^{-1}(\widetilde{M}(\zeta) - Q)R^{-1}$ and, using $\widetilde{M}(i) = Q + iR^2$,

$$M(i) = R^{-1}(Q + iR^2 - Q)R^{-1} = i.$$

□

The reason why the property $M(i) = i$ is so useful is that it allows us to control the norm of Γ. In fact, the following lemma tells us that if $M(i) = i$, then $\|\Gamma\| \leq 1$, i.e. Γ is a contraction.

Lemma 4.1.10. *Let A be a closed symmetric operator on a Hilbert space $\mathfrak{H}$ and let $\Pi = (\mathcal{H}, \Gamma_0, \Gamma_1)$ be a boundary triplet for A^* with Weyl function M satisfying $M(i) = i$. Then*

$$\Gamma : A^* \to \mathcal{H} \oplus \mathcal{H}$$

is a contraction and $\Gamma \restriction \vec{\mathcal{N}}_i \oplus \vec{\mathcal{N}}_{-i}$ is a surjective isometry onto $\mathcal{H} \oplus \mathcal{H}$.

Proof. In principle, the proof works like the proof of [62, Lemma 3.2]. We only have to adapt the statements to the case of linear relations. First note that A^* is a closed subspace of $\mathfrak{H} \oplus \mathfrak{H}$ and the linear relation analog of the von Neumann formula

$$A^* = A \oplus \vec{\mathcal{N}}_i \oplus \vec{\mathcal{N}}_{-i} \tag{4.5}$$

holds (cf. [63, Sect. 2]). Let $\vec{f}_A \in A$ and $\vec{f}_{\pm i} \in \vec{\mathcal{N}}_{\pm i}$. The lemma follows if we prove

$$\|\Gamma(\vec{f}_A + \vec{f}_i + \vec{f}_{-i})\|_{\mathcal{H}^2} = \|\vec{f}_i + \vec{f}_{-i}\|_{\mathfrak{H}^2} \tag{4.6}$$

since $\|\vec{f}_i + \vec{f}_{-i}\|_{\mathfrak{H}^2} \leq \|\vec{f}_A + \vec{f}_i + \vec{f}_{-i}\|_{\mathfrak{H}^2}$. Note that $A = \ker(\Gamma) = \ker(\Gamma_0) \cap \ker(\Gamma_1)$, whence

$$\|\Gamma(\vec{f}_A + \vec{f}_i + \vec{f}_{-i})\|^2_{\mathcal{H}^2} = \|\Gamma_0(\vec{f}_i + \vec{f}_{-i})\|^2_{\mathcal{H}} + \|\Gamma_1(\vec{f}_i + \vec{f}_{-i})\|^2_{\mathcal{H}}. \tag{4.7}$$

Now we proceed with the same calculations as in [62]. For $j \in \{0, 1\}$

$$\|\Gamma_j(\vec{f}_i + \vec{f}_{-i})\|^2_{\mathcal{H}} = \|\Gamma_j \vec{f}_i\|^2_{\mathcal{H}} + 2\Re\mathrm{e}(\langle \Gamma_j \vec{f}_i, \Gamma_j \vec{f}_{-i} \rangle_{\mathcal{H}}) + \|\Gamma_j \vec{f}_{-i}\|^2_{\mathcal{H}}. \tag{4.8}$$

Since $M(i) = i$ by assumption and $M(\overline{z}) = M(z)^*$, we have

$$\Gamma_1 \vec{f}_{\pm i} = M(\pm i)\Gamma_0 f_{\pm i} = \pm i\, \Gamma_0 f_{\pm i}. \tag{4.9}$$

Hence,

$$\|\Gamma_1(\vec{f}_i + \vec{f}_{-i})\|^2_{\mathcal{H}} = \|\Gamma_0 \vec{f}_i\|^2_{\mathcal{H}} - 2\Re\mathrm{e}(\langle \Gamma_0 \vec{f}_i, \Gamma_0 \vec{f}_{-i} \rangle_{\mathcal{H}}) + \|\Gamma_0 \vec{f}_{-i}\|^2_{\mathcal{H}}. \tag{4.10}$$

Adding up (4.8) for $j = 0$ and (4.10), and inserting this into (4.7) gives us

$$\|\Gamma(\vec{f}_A + \vec{f}_i + \vec{f}_{-i})\|^2_{\mathcal{H}^2} = 2(\|\Gamma_0 \vec{f}_i\|^2_{\mathcal{H}} + \|\Gamma_0 \vec{f}_{-i}\|^2_{\mathcal{H}}). \tag{4.11}$$

Using (4.9) and $\vec{f}_{\pm i} = (f_{\pm i}, \pm i f_{\pm i})$, we can use Green's identity

$$\langle \Gamma_1 f_{\pm i}, \Gamma_0 f_{\pm i} \rangle_{\mathcal{H}} - \langle \Gamma_0 f_{\pm i}, \Gamma_1 f_{\pm i} \rangle_{\mathcal{H}} = \langle \pm i f_{\pm i}, f_{\pm i} \rangle_{\mathfrak{H}} - \langle f_{\pm i}, \pm i f_{\pm i} \rangle_{\mathfrak{H}}$$

to obtain

$$\mp i \langle \Gamma_0 \vec{f}_{\pm i}, \Gamma_0 \vec{f}_{\pm i} \rangle_{\mathcal{H}} \mp i \langle \Gamma_0 \vec{f}_{\pm i}, \Gamma_0 \vec{f}_{\pm i} \rangle_{\mathcal{H}} = \mp i \langle f_{\pm i}, f_{\pm i} \rangle_{\mathfrak{H}} \mp i \langle f_{\pm i}, f_{\pm i} \rangle_{\mathfrak{H}}.$$

With $\|\vec{f}_{\pm i}\|^2_{\mathfrak{H}^2} = 2\|f_{\pm i}\|^2_{\mathfrak{H}}$ this gives us $\|\Gamma_0 \vec{f}_{\pm i}\|^2_{\mathcal{H}} = \frac{1}{2}\|\vec{f}_{\pm i}\|^2_{\mathfrak{H}^2}$. Also, since the decomposition (4.5) of A^* is direct, we have $\|\vec{f}_i + \vec{f}_{-i}\|^2_{\mathfrak{H}^2} = \|\vec{f}_i\|^2_{\mathfrak{H}^2} + \|\vec{f}_{-i}\|^2_{\mathfrak{H}^2}$. We insert these two facts into (4.11) to obtain (4.6). Thus, $\Gamma \restriction \vec{\mathcal{N}}_i \oplus \vec{\mathcal{N}}_{-i}$ is an isometry. Since Γ is surjective and $\ker(\Gamma) = A$, the lemma follows. □

With the previous lemma it is simple to prove the following theorem on the direct sum of a sequence of boundary triplets. It was proven by Malamud and Neidhardt [62] for densely defined $A^{(n)}$, $n \in \mathbb{N}_0$, and we state their theorem and its proof in the language of non-densely defined operators and linear relations.

Theorem 4.1.11. *Let $\{A^{(n)}\}_{n\in\mathbb{N}_0}$ be a sequence of closed symmetric operators on separable Hilbert spaces $\mathfrak{H}^{(n)}$. For $n \in \mathbb{N}_0$ let $\Pi^{(n)} = (\mathcal{H}^{(n)}, \Gamma_0^{(n)}, \Gamma_1^{(n)})$ be a boundary triplet for $(A^{(n)})^*$ with Weyl function $M^{(n)}$ and γ-field $\gamma^{(n)}$ such that $M^{(n)}(i) = i$. Furthermore, define $H^{(n)} = \ker(\Gamma_0^{(n)})$ and*

$$A = \bigoplus_{n\in\mathbb{N}_0} A^{(n)}, \qquad H = \bigoplus_{n\in\mathbb{N}_0} H^{(n)}.$$

Then the direct sum Π of the boundary triplets $\{\Pi_n\}_{n\in\mathbb{N}_0}$ given by $\Pi = (\mathcal{H}, \Gamma_0, \Gamma_1)$ with

$$\mathcal{H} = \bigoplus_{n\in\mathbb{N}_0} \mathcal{H}_n, \qquad \Gamma_0 = \bigoplus_{n\in\mathbb{N}_0} \Gamma_0^{(n)}, \qquad \text{and} \qquad \Gamma_1 = \bigoplus_{n\in\mathbb{N}_0} \Gamma_1^{(n)},$$

is a boundary triplet for A^* satisfying $H = \ker(\Gamma_0)$. The Weyl function M and the γ-field γ are given by

$$M(z) = \bigoplus_{n\in\mathbb{N}_0} M^{(n)}(z), \qquad \gamma(z) = \bigoplus_{n\in\mathbb{N}_0} \gamma^{(n)}(z).$$

In particular, M satisfies $M(i) = i$.

Proof. Note that $A^* = \bigoplus_{n\in\mathbb{N}_0} (A^{(n)})^*$. Since $M^{(n)}(i) = i$ for $n \in \mathbb{N}_0$, it follows from Lemma 4.1.10 that $\Gamma^{(n)} = (\Gamma_0^{(n)}, \Gamma_1^{(n)})$ is a contraction for every $n \in \mathbb{N}_0$. This implies

$$\|\Gamma_j\| = \sup_{n\in\mathbb{N}_0} \|\Gamma_j^{(n)}\| \leq 1, \qquad j \in \{0, 1\},$$

whence Γ_0 and Γ_1 are well-defined on A^*. Also,

$$\langle f, g' \rangle - \langle f', g \rangle = \sum_{n\in\mathbb{N}_0} \langle \Gamma_0^{(n)} \vec{f}^{(n)}, \Gamma_1^{(n)} \vec{g}^{(n)} \rangle - \langle \Gamma_1^{(n)} \vec{f}^{(n)}, \Gamma_0^{(n)} \vec{g}^{(n)} \rangle,$$

for $\vec{f}, \vec{g} \in A^*$, $\vec{f} = \{\vec{f}^{(n)}\}_{n\in\mathbb{N}_0}$, $\vec{g} = \{\vec{g}^{(n)}\}_{n\in\mathbb{N}_0}$, whence Green's identity holds. Note that

$$\mathcal{N}_{\pm i} = \ker(A^* \mp i) = \bigoplus_{n\in\mathbb{N}_0} \mathcal{N}_{\pm i}^{(n)}, \qquad \mathcal{N}_{\pm i}^{(n)} = \ker((A^{(n)})^* \mp i).$$

Since $\Gamma^{(n)} \restriction \vec{\mathcal{N}}_i^{(n)} \oplus \vec{\mathcal{N}}_{-i}^{(n)}$ is a surjective isometry onto $\mathcal{H}^{(n)}$ for $n \in \mathbb{N}_0$ by Lemma 4.1.10, $\Gamma = \bigoplus_{n\in\mathbb{N}_0} \Gamma^{(n)}$ is a surjective isometry onto $\mathcal{H}$. Thus, $\Pi = (\mathcal{H}, \Gamma_0, \Gamma_1)$ is a boundary triplet for A^*. The formulae for the Weyl function and the γ-field follow from their definition. Also,

$$H = \bigoplus_{n\in\mathbb{N}_0} H^{(n)} = \bigoplus_{n\in\mathbb{N}_0} \ker(\Gamma_0^{(n)}) = \ker(\Gamma_0).$$

□

4.1.4 A formula for the scattering matrix in terms of the Weyl function

Let us now apply the theory of boundary triplets to derive a formula that expresses the scattering matrix in terms of the Weyl function and the extension parameter B. It is a generalization of a previous result by Behrndt et al. [12], where the theorem was proven for a finite rank coupling, to the case of relatively trace class perturbations.

The general assumptions for this section are as follows. Let H_0 and H be densely defined self-adjoint operators that are bounded from below. Let A be a closed symmetric operator on a Hilbert space $\mathfrak{H}$ with domain $\mathrm{dom}(A) \subset \mathfrak{H}$. It does not have to be densely defined. Furthermore, let $\Pi = (\mathcal{H}, \Gamma_0, \Gamma_1)$ be a boundary triplet for A^* such that $H_0 = \ker(\Gamma_0)$ in the sense of linear relations. Finally, assume that there is a densely defined self-adjoint operator $B \in \mathfrak{L}(\mathcal{H})$ such that $H = \ker(\Gamma_1 - B\Gamma_0)$ and $B^{-1} \in \mathfrak{L}_1(\mathcal{H})$.

As the following lemma shows, with these assumptions we are in the regime of the Landauer-Büttiker formula of Chapter 3 since the scattering system $\{H_0, H\}$ has a resolvent difference that is trace class.

Lemma 4.1.12. *We have* $(H - i)^{-1} - (H_0 - i)^{-1} \in \mathfrak{L}_1(\mathfrak{H})$.

Proof. We know from the Krein-type resolvent formula of Lemma 4.1.8 that

$$(H - i)^{-1} - (H_0 - i)^{-1} = \gamma(i)\big(B - M(i)\big)^{-1}\gamma(-i)^*.$$

Now,

$$\big(B - M(i)\big)^{-1} = |B|^{-\frac{1}{2}}\big(\mathrm{sgn}(B) - |B|^{-\frac{1}{2}}M(i)|B|^{-\frac{1}{2}}\big)^{-1}|B|^{-\frac{1}{2}},$$

where $|B|^{-\frac{1}{2}} \in \mathfrak{L}_2(\mathcal{H})$. But $\big(\mathrm{sgn}(B) - |B|^{-\frac{1}{2}}M(i)|B|^{-\frac{1}{2}}\big)^{-1}$ is bounded since $\Im\mathrm{m}(M(i))$ is boundedly invertible, whence the Lemma follows. □

Note that if $B^{-1} \notin \mathfrak{L}_1(\mathcal{H})$, but only $(B + \theta)^{-1} \in \mathfrak{L}_1(\mathfrak{H})$ for some $\theta \in \mathbb{R}$, we can use the boundary triplet $\widetilde{\Pi} = (\mathcal{H}, \widetilde{\Gamma}_0, \widetilde{\Gamma}_1)$ with

$$\widetilde{\Gamma}_0 = \Gamma_0, \qquad \widetilde{\Gamma}_1 = \Gamma_1 + \theta\Gamma_0.$$

Then

$$\ker(\Gamma_1 - B\Gamma_0) = \ker(\widetilde{\Gamma}_1 - (B + \theta)\widetilde{\Gamma}_0),$$

which implies that the extension parameter $\widetilde{B} = B + \theta$ satisfies our requirements. The Weyl function is then $\widetilde{M}(\zeta) = M(\zeta) + \theta$, whence $B - M(\zeta) = \widetilde{B} - \widetilde{M}(\zeta)$.

It follows from Lemma 4.1.12 that the wave operators $W_\pm(H, H_0)$ exist and are complete by Theorem A.2.9. Thus, the scattering operator $S = W_+^*(H, H_0)W_-(H, H_0)$ is unitary. We introduce the notation

$$R_M(\zeta) = \big(B - M(\zeta)\big)^{-1}, \qquad \zeta \in \rho(H_0).$$

For the proof of our representation of the scattering matrix, we need the following lemma. It is very similar to [11, Lemma 3.2] whose proof we follow closely, but the fact that we take μ to be real not complex changes the result slightly.

Lemma 4.1.13. *For $\mu \in \mathbb{R} \setminus \sigma(H_0)$ and $\lambda \in \mathbb{C} \setminus (\sigma(H) \cup \{\mu\})$, we have*

$$\begin{aligned} &R_M(\mu)\gamma(\mu)^*(H - \lambda)^{-1}\gamma(\mu)R_M(\mu) \\ &\quad = (\lambda - \mu)^{-2}\big(R_M(\mu) - R_M(\lambda)\big) - (\lambda - \mu)^{-1}R_M(\mu)\gamma(\mu)^*\gamma(\mu)R_M(\mu). \end{aligned}$$

Proof. Let $\mu \in \mathbb{R} \setminus \sigma(H_0)$. We start with the resolvent formula

$$(H - \mu)^{-1} = (H_0 - \mu)^{-1} + \gamma(\mu)\big(B - M(\mu)\big)^{-1}\gamma(\mu)^*.$$

Note that $\Gamma_0(H_0 - \mu)^{-1} = 0$ since $\operatorname{ran}((H_0 - \mu)^{-1}) = \operatorname{dom}(H_0) = \ker(\Gamma_0)$. Also, $\Gamma_0\gamma(\mu) = I_{\mathcal{H}}$. We obtain

$$\big(B - M(\mu)\big)^{-1}\gamma(\mu)^* = \Gamma_0(H - \mu)^{-1},$$

whence for $\lambda \in \mathbb{R} \setminus (\sigma(H) \cup \{\mu\})$

$$\begin{aligned} &\big(B - M(\mu)\big)^{-1}\gamma(\mu)^*(H - \lambda)^{-1}\gamma(\mu)\big(B - M(\mu)\big)^{-1} \\ &\quad = \Gamma_0\Big(\big(\Gamma_0(H - \mu)^{-1}(H - \overline{\lambda})^{-1}(H - \mu)^{-1}\big)^*\Big). \end{aligned} \tag{4.12}$$

Note that

$$\begin{aligned} &(H - \mu)^{-1}(H - \overline{\lambda})^{-1}(H - \mu)^{-1} \\ &\quad = (\overline{\lambda} - \mu)^{-1}\big((H - \overline{\lambda})^{-1}(H - \mu)^{-1} - (H - \mu)^{-2}\big) \\ &\quad = (\overline{\lambda} - \mu)^{-2}\big((H - \mu)^{-1} - (H - \overline{\lambda})^{-1}\big) - (\overline{\lambda} - \mu)^{-1}(H - \mu)^{-2}. \end{aligned}$$

Inserting this into (4.12) and using $M(\overline{\lambda})^* = M(\lambda)$ gives us

$$\begin{aligned} &R_M(\mu)\gamma(\mu)^*(H - \lambda)^{-1}\gamma(\mu)R_M(\mu) \\ &= \Gamma_0\Big(\big((\overline{\lambda} - \mu)^{-2}\big(R_M(\mu)\gamma(\mu)^* - R_M(\overline{\lambda})\gamma(\overline{\lambda})^*\big) - (\overline{\lambda} - \mu)^{-1}R_M(\mu)\gamma(\mu)^*(H - \mu)^{-1}\big)^*\Big) \\ &= (\lambda - \mu)^{-2}\big(R_M(\mu) - R_M(\lambda)\big) - (\lambda - \mu)^{-1}R_M(\mu)\gamma(\mu)^*\gamma(\mu)R_M(\mu) \end{aligned}$$

□

Now we choose the spectral representation with respect to which we want to calculate $S(\lambda)$. Note that

$$\varphi : (\zeta_0, \infty) \to \mathbb{R}, \qquad \varphi(\mu) = -(\mu + \zeta_0)^{-1},$$

is admissible in the invariance principle for wave operators, cf. Theorem A.2.12, whence $W_\pm(H, H_0) = W_\pm(\varphi(H), \varphi(H_0))$. Let $K_0 = \varphi(H_0)$ and $K = \varphi(H)$. Then

$$\begin{aligned} V = K - K_0 &= -\gamma(\zeta_0)\big(B - M(-\zeta_0)\big)^{-1}\gamma(-\zeta_0)^* \\ &= -\gamma(-\zeta_0)|B|^{-\frac{1}{2}}\big(\operatorname{sgn}(B) - |B|^{-\frac{1}{2}}M(-\zeta_0)|B|^{-\frac{1}{2}}\big)^{-1}|B|^{-\frac{1}{2}}\gamma(-\zeta_0)^*. \end{aligned} \tag{4.13}$$

Let $C = \gamma(-\zeta_0)|B|^{-\frac{1}{2}} \in \mathfrak{L}_2(\mathcal{H}, \mathfrak{H})$. Let $X : \mathbb{R} \to \mathfrak{B}(\mathcal{H})$ be strongly continuous and let the operator spectral integrals below exist. Then Lemma 3.1.4 gives us a spectral representation Φ_{H_0} of H_0^{ac} satisfying

$$\Big(\Phi_{H_0}\int_{\mathbb{R}} \mathrm{d}E_{H_0}^{ac}(\mu)CX(\mu)f\Big)(\lambda) = \sqrt{Y_{\zeta_0}(\lambda)}X(\lambda)f, \qquad f \in \mathcal{H},$$

and

$$\int_{\mathbb{R}} X(\mu)C^*\mathrm{d}E_{H_0}^{ac}(\mu)\Phi_{H_0}^*\widehat{f} = \int_{\mathbb{R}} \mathrm{d}\mu\, X(\mu)\sqrt{Y_{\zeta_0}(\mu)}\widehat{f}(\mu), \qquad \widehat{f} = \Phi_{H_0}^* f,$$

where

$$Y_{\zeta_0}(\lambda) = \frac{\mathrm{d}}{\mathrm{d}\lambda}C^*E_{H_0}(\lambda)C, \tag{4.14}$$

using [9, Prop. I.3.13]. We introduce the notation

$$M_B(-\zeta) = |B|^{-\frac{1}{2}}M(-\zeta)|B|^{-\frac{1}{2}}, \qquad R_{M_B}(\zeta) = (\operatorname{sgn}(B) - M_B(\zeta))^{-1}, \qquad \zeta \in \rho(H_0).$$

We can prove the following representation of the scattering matrix, which generalizes the result of Behrndt et al. [12] to relatively trace class perturbations.

Theorem 4.1.14. *For a.e. $\lambda \in \mathbb{R}$ the scattering matrix admits the representation*

$$S(\lambda) = 1 + 2i\,\Im\mathrm{m}\big(M_B(\lambda)\big)^{\frac{1}{2}}\big(\operatorname{sgn}(B) - M_B(\lambda)\big)^{-1}\Im\mathrm{m}\big(M_B(\lambda)\big)^{\frac{1}{2}}$$

with respect to the spectral representation Φ_{H_0}.

Proof. Note that $V = CR_{M_B}(\zeta_0)C^*$. With respect to the spectral representation Φ_{K_0} constructed from $Y_{K_0}(\lambda) = \frac{\mathrm{d}}{\mathrm{d}\lambda}C^*E_{K_0}(\lambda)C$, Proposition 3.1.6 gives us

$$\check{T}(\lambda) = \lim_{\epsilon\to+0}\sqrt{Y_{K_0}(\lambda)}\big(R_{M_B}(\zeta_0) - R_{M_B}(\zeta_0)C^*(K - \lambda - i\epsilon)^{-1}CR_{M_B}(\zeta_0)\big)\sqrt{Y_{K_0}(\lambda)}$$

for a.e. $\lambda \in \mathbb{R}$, where $S = P_{H_0}^{ac} - 2\pi i\, T$. Let $\varphi(\lambda) = -(\lambda+\zeta_0)^{-1}$ and $\varphi^{-1}(\lambda) = -\lambda^{-1} - \zeta_0$, i.e. $\varphi(\varphi^{-1}(\lambda)) = \lambda$. Then $E_{K_0}(\lambda) = E_{H_0}(\varphi^{-1}(\lambda))$ and $T(\lambda) = \check{T}(\varphi(\lambda))$ (cf. the proof of Theorem 3.1.2). We have

$$Y_{K_0}(\varphi(\lambda)) = (\varphi^{-1})'(\varphi(\lambda))\frac{\mathrm{d}}{\mathrm{d}\lambda}C^*E_{H_0}\big(\varphi^{-1}(\varphi(\lambda))\big)C = (\lambda + \zeta_0)^2 Y_{\zeta_0}(\lambda).$$

Also,

$$\begin{aligned}(K-\varphi(\lambda)-i\epsilon)^{-1} &= (H+\zeta_0)\big(-1-(\varphi(\lambda)+i\epsilon)(H+\zeta_0)\big)^{-1}\\ &= -(H+\zeta_0)(\varphi(\lambda)+i\epsilon)^{-1}\big(H+\zeta_0+(\varphi(\lambda)+i\epsilon)^{-1}\big)^{-1}\\ &= (\varphi(\lambda)+i\epsilon)^{-2}\big(H+\zeta_0+(\varphi(\lambda)+i\epsilon)^{-1}\big)^{-1}-(\varphi(\lambda)+i\epsilon)^{-1}\end{aligned}$$

and

$$\lim_{\epsilon\to+0}(\varphi(\lambda)+i\epsilon)^{-1} = \lim_{\epsilon\to+0}\frac{-(\lambda+\zeta_0)^{-1}}{(\lambda+\zeta_0)^{-2}+\epsilon^2} - i\frac{\epsilon}{(\lambda+\zeta_0)^{-2}+\epsilon^2} = -\lambda-\zeta_0-i0.$$

Hence, we obtain

$$\begin{aligned}T(\lambda) = (\lambda+\zeta_0)^2&\sqrt{Y_{\zeta_0}(\lambda)}R_{M_B}(\zeta_0)\sqrt{Y_{\zeta_0}(\lambda)}\\ &+\sqrt{Y_{\zeta_0}(\lambda)}R_{M_B}(\zeta_0)C^*CR_{M_B}(\zeta_0)\sqrt{Y_{\zeta_0}(\lambda)}(\lambda+\zeta_0)^3\\ &+(\lambda+\zeta_0)^4\sqrt{Y_{\zeta_0}(\lambda)}R_{M_B}(\zeta_0)C^*(H-\lambda-i0)^{-1}CR_{M_B}(\zeta_0)\sqrt{Y_{\zeta_0}(\lambda)}\end{aligned}$$

for a.e. $\lambda\in\mathbb{R}$. Now we want to express the individual summands in terms of the Weyl function. We proceed as in the proof of [12, Thm. 3.1]. The formula

$$\Im\mathrm{m}(M(\lambda+i\epsilon)) = \epsilon\gamma(\lambda+i\epsilon)^*\gamma(\lambda+i\epsilon)$$

together with the identity

$$\begin{aligned}\gamma(\lambda+i\epsilon) &= (1+(\lambda+\zeta_0+i\epsilon)(H_0-\lambda-i\epsilon)^{-1})\gamma(-\zeta_0)\\ &= (H_0+\zeta_0)(H_0-\lambda-i\epsilon)^{-1}\gamma(-\zeta_0)\end{aligned}$$

amounts to

$$\begin{aligned}\Im\mathrm{m}(M(\lambda+i\epsilon)) &= \epsilon\,\gamma(-\zeta_0)^*(H_0+\zeta_0)^2(H_0-\lambda-i\epsilon)^{-1}(H_0-\lambda+i\epsilon)^{-1}\gamma(-\zeta_0)\\ &= (2i)^{-1}\gamma(-\zeta_0)^*(H_0+\zeta_0)^2\big((H_0-\lambda-i\epsilon)^{-1}-(H_0-\lambda+i\epsilon)^{-1}\big)\gamma(-\zeta_0).\end{aligned}$$

Now, [9, Prop. I.3.14] states that

$$C^*\big((H_0-\lambda-i0)^{-1}-(H_0-\lambda+i0)^{-1}\big)C = 2\pi i\frac{\mathrm{d}}{\mathrm{d}\lambda}C^*E_{H_0}(\lambda)C \equiv 2\pi i Y_{\zeta_0}(\lambda)$$

for a.e. $\lambda\in\mathbb{R}$. We obtain

$$\Im\mathrm{m}\big(M_B(\lambda)\big) = \lim_{\epsilon\to+0}|B|^{-\frac{1}{2}}\Im\mathrm{m}\big(M(\lambda+i\epsilon)\big)|B|^{-\frac{1}{2}} = \pi(\lambda+\zeta_0)^2Y_{\zeta_0}(\lambda). \tag{4.15}$$

This gives us

$$\sqrt{Y_{\zeta_0}(\lambda)} = \pi^{-\frac{1}{2}}|\lambda+\zeta_0|^{-1}\Im\mathrm{m}\big(M_B(\lambda)\big)^{\frac{1}{2}}.$$

Lemma 4.1.13 implies that

$$\begin{aligned}
&(\operatorname{sgn}(B) - M_B(\zeta_0))^{-1}|B|^{-\frac{1}{2}}\gamma(\zeta_0)^*(H-\lambda+i\epsilon)^{-1}\gamma(\zeta_0)^*|B|^{-\frac{1}{2}}(\operatorname{sgn}(B) - M_B(\zeta_0))^{-1}\\
&\quad = (\lambda+i\epsilon+\zeta_0)^{-2}|B|^{\frac{1}{2}}\big(R_M(-\zeta_0) - R_M(\lambda)\big)|B|^{\frac{1}{2}}\\
&\qquad\qquad - (\lambda+i\epsilon+\zeta_0)^{-1}|B|^{\frac{1}{2}}R_M(-\zeta_0)\gamma(-\zeta_0)^*\gamma(-\zeta_0)R_M(-\zeta_0)|B|^{\frac{1}{2}}\\
&\quad = (\lambda+i\epsilon+\zeta_0)^{-2}\big(R_{M_B}(-\zeta_0) - R_{M_B}(\lambda)\big)\\
&\qquad\qquad - (\lambda+i\epsilon+\zeta_0)^{-1}R_{M_B}(-\zeta_0)|B|^{-\frac{1}{2}}\gamma(-\zeta_0)^*\gamma(-\zeta_0)|B|^{-\frac{1}{2}}R_{M_B}(-\zeta_0).
\end{aligned}$$

We arrive at

$$\begin{aligned}
\pi\, T(\lambda) =& -\Im\mathrm{m}\big(M_B(\lambda)\big)^{\frac{1}{2}}R_{M_B}(-\zeta_0)\Im\mathrm{m}\big(M_B(\lambda)\big)^{\frac{1}{2}}\\
&+(\lambda+\zeta_0)\Im\mathrm{m}\big(M_B(\lambda)\big)^{\frac{1}{2}}R_{M_B}(-\zeta_0)C^*CR_{M_B}(-\zeta_0)\Im\mathrm{m}\big(M_B(\lambda)\big)^{\frac{1}{2}}\\
&+\Im\mathrm{m}\big(M_B(\lambda)\big)^{\frac{1}{2}}\big(R_{M_B}(-\zeta_0) - R_{M_B}(\lambda)\big)\Im\mathrm{m}\big(M_B(\lambda)\big)^{\frac{1}{2}}\\
&-(\lambda+\zeta_0)\Im\mathrm{m}\big(M_B(\lambda)\big)^{\frac{1}{2}}R_{M_B}(-\zeta_0)C^*CR_{M_B}(-\zeta_0)\Im\mathrm{m}\big(M_B(\lambda)\big)^{\frac{1}{2}}\\
=& -\Im\mathrm{m}\big(M_B(\lambda)\big)^{\frac{1}{2}}\big(\operatorname{sgn}(B) - M_B(\lambda)\big)^{-1}\Im\mathrm{m}\big(M_B(\lambda)\big)^{\frac{1}{2}}.
\end{aligned}$$

□

Theorem 4.1.14 does not have exactly the same form as the corresponding result for finite-dimensional perturbations since it expresses the scattering matrix in terms of $M_B(\lambda)$ and not of $M(\lambda)$. The fact that the limit $M_B(\lambda+i0) = |B|^{-\frac{1}{2}}M(\lambda+i0)|B|^{-\frac{1}{2}}$ in (4.15) exists is due to the Hilbert-Schmidt property of $|B|^{-\frac{1}{2}}$. The following corollary shows that if the limits $M(\lambda+i0)$ exist without the operators $|B|^{-\frac{1}{2}}$, we obtain the same formula as in the finite dimensional case.

Corollary 4.1.15. *If the limits $M(\lambda) = \text{s-}\lim_{\epsilon\to+0} M(\lambda+i\epsilon)$ exist for a.e. $\lambda\in\mathbb{R}$, the scattering matrix admits the representation*

$$S(\lambda) = 1 + 2i\,\Im\mathrm{m}\big(M(\lambda)\big)^{\frac{1}{2}}\big(B - M(\lambda)\big)^{-1}\Im\mathrm{m}\big(M(\lambda)\big)^{\frac{1}{2}}$$

for a.e. $\lambda\in\mathbb{R}$ with respect to the spectral representation $\widetilde{\Phi}_{H_0} = \widetilde{U}\Phi_{H_0}$ of H_0^{ac}. Here, $\widetilde{U}$ is some unitary operator $\widetilde{U}: L^2(\mathbb{R},\mathrm{d}\lambda,\mathfrak{H}_\lambda)\to L^2(\mathbb{R},\mathrm{d}\lambda,\mathcal{H}_{fin}(\lambda))$ with

$$\mathcal{H}_{fin}(\lambda) = \mathrm{clo}\Big(\mathrm{ran}\Big(\Im\mathrm{m}(M(\lambda))\Big)\Big).$$

Proof. Since $M_B(\lambda) = |B|^{-\frac{1}{2}}M(\lambda)|B|^{-\frac{1}{2}}$ and $|B|^{-\frac{1}{2}}\in\mathfrak{L}_2(\mathcal{H})$, the imaginary part satisfies

$$\Im\mathrm{m}\big(M_B(\lambda)\big) = \lim_{\epsilon\to+0}|B|^{-\frac{1}{2}}\Im\mathrm{m}\big(M(\lambda+i\epsilon)\big)|B|^{-\frac{1}{2}},$$

where the limit is taken in the trace norm. For a.e. $\lambda\in\mathbb{R}$ the polar decomposition gives us

$$\Im\mathrm{m}\big(M_B(\lambda)\big)^{\frac{1}{2}} = U^*(\lambda)\Im\mathrm{m}\big(M(\lambda)\big)^{\frac{1}{2}}|B|^{-\frac{1}{2}}$$

for some partial isometry $U(\lambda)$ with initial space

$$\mathcal{H}_{ini}(\lambda) = \mathrm{clo}\Big(\mathrm{ran}\Big(|B|^{-\frac{1}{2}}\Im\mathrm{m}(M(\lambda))^{\frac{1}{2}}\Big)\Big)$$

and final space

$$\mathcal{H}_{fin}(\lambda) = \mathrm{clo}\Big(\mathrm{ran}\Big(\Im\mathrm{m}(M(\lambda))^{\frac{1}{2}}|B|^{-\frac{1}{2}}\Big)\Big) = \mathrm{clo}\Big(\mathrm{ran}\Big(\Im\mathrm{m}(M(\lambda))^{\frac{1}{2}}\Big)\Big).$$

We obtain

$$T(\lambda) = -\pi^{-1}U^*(\lambda)\Im\mathrm{m}(M(\lambda))^{\frac{1}{2}}|B|^{-\frac{1}{2}}R_{M_B}(\lambda)|B|^{-\frac{1}{2}}\Im\mathrm{m}(M(\lambda))^{\frac{1}{2}}U(\lambda).$$

Recall from Lemma 3.1.4 that Φ_{H_0} maps $\mathfrak{H}$ onto $L^2(\mathbb{R}, \mathrm{d}\lambda, \mathfrak{H}_\lambda)$, where

$$\mathfrak{H}_\lambda = \mathrm{clo}\Big(\mathrm{ran}\Big(Y(\lambda)\Big)\Big) = \mathrm{clo}\Big(\mathrm{ran}\Big(\sqrt{Y(\lambda)}\Big)\Big)$$

with $Y(\lambda) = \frac{\mathrm{d}}{\mathrm{d}\lambda}CE_{H_0}(\lambda)C^* \geq 0$. Thus, in our case $\mathcal{H}_{fin}(\lambda) = \mathrm{clo}(\mathrm{ran}(\Im\mathrm{m}(M(\lambda))))$ and

$$\begin{aligned}\mathfrak{H}_\lambda = \mathrm{clo}\Big(\mathrm{ran}\Big(\Im\mathrm{m}(M_B(\lambda))\Big)\Big) &= \mathrm{clo}\Big(\mathrm{ran}\Big(\Im\mathrm{m}(M_B(\lambda))^{\frac{1}{2}}\Big)\Big)\\ &= \mathrm{clo}\Big(\mathrm{ran}\Big(|B|^{-\frac{1}{2}}\Im\mathrm{m}(M(\lambda))^{\frac{1}{2}}\Big)\Big),\end{aligned}$$

whence $\mathfrak{H}_\lambda = \mathcal{H}_{ini}(\lambda)$. Let $\widetilde{U}(\lambda)$ be an isometry such that $U(\lambda) = \widetilde{U}(\lambda) \restriction \mathcal{H}_{fin}(\lambda)$. It satisfies $\widetilde{U}^*(\lambda)U(\lambda) = P_{\mathcal{H}_{fin}(\lambda)}$. We define

$$\widetilde{U} : L^2(\mathbb{R}, \mathrm{d}\lambda, \mathcal{H}_{fin}(\lambda)) \to L^2(\mathbb{R}, \mathrm{d}\lambda, \mathfrak{H}_\lambda), \qquad (\widetilde{U}f) = \widetilde{U}(\lambda)f(\lambda),$$

which is also an isometry. Then we may take $T(\lambda)$ with respect to the spectral representation $\widetilde{U}\Phi_{H_0}$. It follows that

$$\begin{aligned}T(\lambda) &= -\pi^{-1}P_{\mathcal{H}_{fin}(\lambda)}\Im\mathrm{m}(M(\lambda))^{\frac{1}{2}}|B|^{-\frac{1}{2}}R_{M_B}(\lambda)|B|^{-\frac{1}{2}}\Im\mathrm{m}(M(\lambda))^{\frac{1}{2}}P_{\mathcal{H}_{fin}(\lambda)}\\ &= -\pi^{-1}\,\Im\mathrm{m}(M(\lambda))^{\frac{1}{2}}(B - M(\lambda))^{-1}\Im\mathrm{m}(M(\lambda))^{\frac{1}{2}}.\end{aligned}$$

□

4.2 A boundary triplet for the Jaynes-Cummings quantum dot LED

In this section we use the theory of boundary triplets for non-densely defined closed symmetric operators to define a boundary triplet for the QD-LED based on the Jaynes-Cummings model we presented in Section 3.2. It allows us to use Theorem 4.1.14 to obtain a formula for the scattering matrix in terms of the Weyl function and the extension parameter. We construct the boundary triplet for $A^* \supset H_0$ as a direct sum of boundary triplets using Theorem 4.1.11. We use the spectral decompositions $H_j = \bigoplus_{n\in\mathbb{N}_0} H_j^{(n)}$, $j \in \{l, S, r\}$, of the Hamiltonians of the leads and the quantum dot and construct

boundary triplets for each summand $H_j^{(n)}$. We start with a boundary triplet for the purely electric model without the photon field since it uses a construction that we also use for the full model and helps us to find the correct extension parameter.

4.2.1 The electric model

Recall that the electric part of the Jaynes-Cummings QD-LED lives on the Hilbert space $\mathfrak{h}^{el} = \mathfrak{h}_l^{el} \oplus \mathfrak{h}_S^{el} \oplus \mathfrak{h}_r^{el}$ with $\mathfrak{h}_j^{el} = \ell^2(\mathbb{N}_0)$, $j \in \{l, r\}$, for the leads, and $\mathfrak{h}_S^{el} = \mathbb{C}^d$ for some $d \geq 2$ for the quantum dot. The Hamiltonian h_0^{el} for decoupled leads is

$$h_0^{el} = h_l^{el} \oplus h_S^{el} \oplus h_r^{el}, \qquad h_j^{el} = -\Delta^D + v_j, \qquad h_S^{el} = (h_S^{el})^* \in \mathbb{C}^{d\times d}, \qquad j \in \{l, r\},$$

where Δ^D denotes the discrete Laplacian on $\ell^2(\mathbb{N})$ with homogeneous Dirichlet boundary condition and h_S^{el} is some $d\times d$-matrix with eigenvectors e_m for eigenvalues $\lambda_m = v_0 + m\omega_0$, $0 \leq m \leq d-1$. Note that all operators are bounded. Let $x_j^1 \in \mathfrak{h}_j^{el}$ denote the vector $x_j^1 = (1, 0, 0, \ldots) \in \ell^2(\mathbb{N})$, $j \in \{l, r\}$. Let $\{x_S^0, \ldots, x_S^{d-1}\}$ be a basis of $\mathfrak{h}_S^{el}$, where x_S^0 and x_S^{d-1} are the left respectively right contact points of the quantum dot. We can define the Hilbert spaces

$$\mathcal{H}^{el} = \mathcal{H}_l^{el} \oplus \mathcal{H}_S^{el} \oplus \mathcal{H}_r^{el}, \qquad \mathcal{H}_l^{el} = \mathbb{C}x_l^1, \quad \mathcal{H}_r^{el} = \mathbb{C}x_r^1, \quad \mathcal{H}_S^{el} = \mathbb{C}x_S^0 \oplus \mathbb{C}x_S^{d-1},$$

which gives us the decomposition

$$\mathfrak{h}^{el} = (\mathcal{H}^{el})^\perp \oplus \mathcal{H}^{el}, \qquad (\mathcal{H}^{el})^\perp = \ell^2(\mathbb{N} \setminus \{1\}) \oplus \operatorname{span}(\{x_S^1, \ldots, x_S^{d-2}\}) \oplus \ell^2(\mathbb{N} \setminus \{1\}).$$

With respect to this decomposition of $\mathfrak{h}^{el}$, we can write the coupling of the leads as

$$v_{el} = 0 \oplus \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \qquad h^{el} = h_0^{el} + \tau_{el} v_{el}.$$

Note in particular that $P_{\mathcal{H}^{el}} v_{el} \upharpoonright \mathcal{H}^{el}$ is invertible, where $P_{\mathcal{H}^{el}}$ is the orthogonal projection of $\mathfrak{h}^{el}$ onto $\mathcal{H}^{el}$. Now, we want to find closed symmetric operators A_j^{el}, $j \in \{l, S, r\}$, such that both h_0^{el} and h^{el} are extensions of $A^{el} = A_l^{el} \oplus A_S^{el} \oplus A_r^{el}$. From the definition of v_{el}, it is obvious that

$$A_j^{el} = h_j^{el} \upharpoonright \operatorname{dom}(A_j^{el}), \qquad \operatorname{dom}(A_j^{el}) = (\mathcal{H}_j^{el})^\perp, \qquad j \in \{l, S, r\},$$

are such operators. Since h_j^{el} is bounded for $j \in \{l, S, r\}$, we have

$$(A_j^{el})^* = \{(f_j^{el}, h_j^{el} f_j^{el} + y_j^{el}) \mid f_j^{el} \in \mathfrak{h}_j^{el}, y_j^{el} \in \mathcal{H}_j^{el}\}$$

as a linear relation on $\mathfrak{h}_j^{el}$. This implies

$$(A^{el})^* = \{(f^{el}, h_0^{el} f^{el} + y^{el}) \mid f^{el} \in \mathfrak{h}^{el}, y^{el} \in \mathcal{H}^{el}\}.$$

It is important to note that this holds only since h_0^{el} is bounded. If h_0^{el} were unbounded, we would have to choose $f^{el} \in \mathrm{dom}(h_0^{el})$. In the following lemma we explicitly construct boundary triplets for h_j^{el}, $j \in \{l, S, r\}$.

Lemma 4.2.1. *For $j \in \{l, S, r\}$ the triplet $\Pi_j^{el} = (\mathcal{H}_j^{el}, \Gamma_{0,j}^{el}, \Gamma_{1,j}^{el})$ with*

$$\Gamma_{0,j}^{el} \vec{f}_j^{el} = y_j^{el}, \qquad \Gamma_{1,j}^{el} \vec{f}_j^{el} = -P_{\mathcal{H}_j^{el}} f_j^{el}, \qquad \vec{f}_j^{el} = (f_j^{el}, h_j^{el} f_j^{el} + y_j^{el}) \in (A_j^{el})^*,$$

is a boundary triplet for $(A_j^{el})^*$ with γ-field and Weyl function

$$\gamma_j^{el}(\zeta) = -(h_j^{el} - \zeta)^{-1} \restriction \mathcal{H}_j^{el} \qquad \text{and} \qquad M_j^{el}(\zeta) = P_{\mathcal{H}_j^{el}} (h_j^{el} - \zeta)^{-1} \restriction \mathcal{H}_j^{el},$$

respectively. It satisfies $A_j^{el} = \ker(\Gamma_{0,j}^{el})$.

Proof. Let $j \in \{l, S, r\}$. Since $f_j^{el} \in \mathfrak{h}_j^{el}$ and $y_j^{el} \in \mathcal{H}_j^{el}$ are arbitrary, the surjectivity of $\Gamma_j^{el} = (\Gamma_{0,j}^{el}, \Gamma_{1,j}^{el})$ is obvious. To show that Π_j^{el} is a boundary triplet, it remains to check that Green's identity holds. For $\vec{f}_j^{el}, \vec{g}_j^{el} \in (A_j^{el})^*$ with $\vec{f}_j^{el} = (f_j^{el}, h_j^{el} f_j^{el} + y_j^{el})$ and $\vec{g}_j^{el} = (g_j^{el}, h_j^{el} g_j^{el} + z_j^{el})$, we have

$$\begin{aligned}
&\langle f_j^{el}, h_j^{el} g_j^{el} + z_j^{el} \rangle - \langle h_j^{el} f_j^{el} + y_j^{el}, g_j^{el} \rangle \\
&\quad = \langle f_j^{el}, h_j^{el} g_j^{el} \rangle - \langle f_j^{el}, h_j^{el} g_j^{el} \rangle + \langle P_{\mathcal{H}_j^{el}} f_j^{el}, z_j^{el} \rangle - \langle y_j^{el}, P_{\mathcal{H}_j^{el}} g_j^{el} \rangle \\
&\quad = \langle \Gamma_{0,j}^{el} \vec{f}_j^{el}, \Gamma_{1,j}^{el} \vec{g}_j^{el} \rangle - \langle \Gamma_{1,j}^{el} \vec{f}_j^{el}, \Gamma_{0,j}^{el} \vec{g}_j^{el} \rangle.
\end{aligned}$$

Let $\zeta \in \rho(h_j^{el})$. Note that $f_j^{el}(\zeta) \in \ker((A_j^{el})^* - \zeta)$ if and only if

$$f_j^{el}(\zeta) = -(h_j^{el} - \zeta)^{-1} y_j^{el}$$

for some $y_j^{el} \in \mathcal{H}_j^{el}$. Also,

$$\zeta f_j^{el}(\zeta) = -\zeta (h_j^{el} - \zeta)^{-1} y_j^{el} = -h_j^{el} (h_j^{el} - \zeta)^{-1} y_j^{el} + y_j^{el} = h_j^{el} f_j^{el}(\zeta) + y_j^{el}.$$

Hence, for

$$\vec{f}_j^{el}(\zeta) = (-(h_j^{el} - \zeta)^{-1} y_j^{el}, -\zeta (h_j^{el} - \zeta)^{-1} y_j^{el}) \in \vec{\mathcal{N}}_{j,\zeta}^{el},$$

we obtain $\Gamma_{0,j}^{el} \vec{f}_j^{el}(\zeta) = y_j^{el}$, which results in

$$\gamma_j^{el}(\zeta) = P_{\mathfrak{h}_j^{el}}^1 (\Gamma_{0,j}^{el} \restriction \vec{\mathcal{N}}_{j,\zeta}^{el})^{-1} = -(h_j^{el} - \zeta)^{-1} \restriction \mathcal{H}_j^{el}$$

and

$$M_j^{el}(\zeta) = \Gamma_1 (\Gamma_{0,j}^{el} \restriction \vec{\mathcal{N}}_{j,\zeta}^{el})^{-1} = P_{\mathcal{H}_j^{el}} (h_j^{el} - \zeta)^{-1} \restriction \mathcal{H}_j^{el}.$$

Finally, $\vec{f}_j^{el} = (f_j^{el}, h_j^{el} f_j^{el} + y_j^{el}) \in \ker(\Gamma_{0,j}^{el})$ if and only if $y_j^{el} = 0$. But this implies

$$\ker(\Gamma_{0,j}^{el}) = \{(f_j^{el}, h_j^{el} f_j^{el}) \,|\, f_j^{el} \in \mathfrak{h}_j^{el}\} = h_j^{el}$$

in the sense of linear relations. □

Remark 4.2.2. *We see from the proof that the boundedness of h_j^{el} is needed for the surjectivity of Γ_1. If h_j^{el} were unbounded, the fact that $f_j^{el} \in \mathrm{dom}(h_j^{el}) \subsetneq \mathfrak{h}_j^{el}$ would imply that $\Gamma_1 f_j^{el} = -P_{\mathcal{H}_j^{el}} f_j^{el}$ would not be surjective.*

We can combine the boundary triplets of Lemma 4.2.1 to obtain a boundary triplet Π^{el} for $(A^{el})^*$ given by

$$\Pi^{el} = (\mathcal{H}^{el}, \Gamma_0^{el}, \Gamma_1^{el}) = \Pi_l^{el} \oplus \Pi_S^{el} \oplus \Pi_r^{el}.$$

Obviously, it satisfies $\ker(\Gamma_0^{el}) = h_0^{el}$ and

$$\gamma^{el}(\zeta) = -(h_0^{el} - \zeta)^{-1} \restriction \mathcal{H}^{el}, \qquad M^{el}(\zeta) = P_{\mathcal{H}^{el}}(h_0^{el} - \zeta)^{-1} \restriction \mathcal{H}^{el}.$$

To express the scattering system $\{h_0^{el}, h^{el}\}$ in terms of boundary triplets, it remains to specify the correct extension parameter B^{el}. This is done in the following Lemma.

Lemma 4.2.3. *The extension parameter $B^{el} = -(P_{\mathcal{H}^{el}} \tau_{el} v_{el} \restriction \mathcal{H}^{el})^{-1}$ gives*

$$h^{el} = \ker(\Gamma_1^{el} - B^{el}\Gamma_0^{el}).$$

Proof. Let $\vec{f}^{el} = (f^{el}, h_0^{el} f^{el} + y^{el}) \in (A^{el})^*$. Then

$$-P_{\mathcal{H}^{el}} f^{el} = \Gamma_1^{el} \vec{f}^{el} = B^{el}\Gamma_0^{el} \vec{f}^{el} = B^{el} y^{el}$$

implies $y^{el} = \tau_{el} v_{el} f^{el}$. This gives us

$$\ker(\Gamma_1^{el} - B^{el}\Gamma_0^{el}) = \{(f^{el}, (h_0^{el} + \tau_{el} v_{el}) f^{el}) \,|\, f^{el} \in \mathfrak{h}^{el}\} = h^{el}.$$

□

Theorem 4.1.14 immediately gives us the scattering matrix. Note that in this case B^{el} is a finite rank operator, whence the finite rank version of the proposition that can be found in [12] is sufficient. Since the limits $M^{el}(\lambda + i0)$ exist, this is equivalent to Corollary 4.1.15, which gives us

$$s^{el}(\lambda) = 1 + 2i\,\Im\mathrm{m}(M^{el}(\lambda))^{\frac{1}{2}}(B^{el} - M^{el}(\lambda))^{-1}\Im\mathrm{m}(M^{el}(\lambda))^{\frac{1}{2}}. \tag{4.16}$$

This expresses the scattering matrix in terms of the explicitly known extension parameter B^{el} and the Weyl function, which in our case is nothing but a projection of the resolvent of h_0^{el}. Recall from Lemma 3.2.2 that we know the eigenfunctions, and hence the resolvent, of h_j^{el}, $j \in \{l, r\}$. In fact,

$$M_j^{el}(\lambda + i\epsilon) = \int_{\mathbb{R}} \mathrm{d}\mu |g_j(1,\mu)|^2 (\mu - \lambda - i\epsilon)^{-1}.$$

Using Lemma A.2.20, we obtain

$$M_j^{el}(\lambda) = \lim_{\epsilon \to +0} \int_{|\lambda - \mu| > \epsilon} \mathrm{d}\mu |g_j(1,\mu)|^2 (\mu - \lambda)^{-1} + i\pi\,|g_j(1,\lambda)|^2.$$

Since h_S^{el} is a finite-dimensional matrix, the calculation of the resolvent of h_S^{el} is straightforward. Thus, the scattering matrix can be calculated explicitly with formula (4.16).

4.2.2 The full model

We want to use the construction of the previous section to construct a boundary triplet for the full model of a QD-LED based on the generalized Jaynes-Cummings model (cf. Section 3.2). We want to apply Theorem 4.1.14 to this boundary triplet to get an explicit formula for the scattering matrix, which can then be used in the Landauer-Büttiker formula of Theorem 3.1.2.

Recall that the Hamiltonians of the leads are $H_j = h_j^{el} \otimes I_{ph} + I_{\mathfrak{h}_j^{el}} \otimes h^{ph}$, $j \in \{l, S, r\}$, where the photon Hamiltonian is $h^{ph} = \omega\, a^* a$ on $\mathfrak{h}^{ph} = \mathfrak{F}_+(\mathbb{C}) = \ell^2(\mathbb{N}_0)$ with eigenvectors Υ_n satisfying $h^{ph}\Upsilon_n = n\omega\Upsilon_n$, $n \in \mathbb{N}_0$. We can write this as

$$H_j = \bigoplus_{n\in\mathbb{N}_0} H_j^{(n)}, \qquad H_j^{(n)} = h_j^{el} + n\omega,$$

with $H_j^{(n)}$ acting on $\mathfrak{H}_j^{(n)} = \mathfrak{h}_j^{el} \otimes \mathbb{C}\Upsilon_n$, $n \in \mathbb{N}_0$. Just as in the previous section, for $n \in \mathbb{N}_0$ we set

$$\mathcal{H}_l^{(n)} = \mathcal{H}_l^{el} \otimes \mathbb{C}\Upsilon_n = \mathbb{C}(x_l^1 \otimes \Upsilon_n) \qquad \text{and} \qquad \mathcal{H}_r^{(n)} = \mathcal{H}_r^{el} \otimes \mathbb{C}\Upsilon_n = \mathbb{C}(x_r^1 \otimes \Upsilon_n).$$

For the quantum dot we choose

$$\mathcal{H}_S^{(n)} = \mathfrak{h}_S^{el} \otimes \mathbb{C}\Upsilon_n.$$

This choice of $\mathcal{H}_S^{(n)}$ as the whole space comes from the fact that $\mathrm{clo}(\mathrm{ran}(V_{int})) = \mathfrak{H}_S$. Thus, it is not sufficient to only use the contact points of the quantum dot $\mathcal{H}_S^{el} \otimes \mathbb{C}\Upsilon_n$ as the boundary value space. We obtain the non-densely defined closed symmetric operators

$$A_j^{(n)} = H_j^{(n)} \restriction \mathrm{dom}(A_j^{(n)}), \qquad \mathrm{dom}(A_j^{(n)}) = (\mathcal{H}_j^{(n)})^{\perp},$$

where $A_S^{(n)} = \{(0,0)\}$ is actually the null operator with the null space as domain. The adjoint is

$$(A_j^{(n)})^* = \{(f_j^{(n)}, H_j^{(n)} f_j^{(n)} + y_j^{(n)}) \,|\, f_j^{(n)} \in \mathfrak{H}_j^{(n)}, y_j^{(n)} \in \mathcal{H}_j^{(n)}\}. \tag{4.17}$$

Remark 4.2.4. *The representation* (4.17) *holds since $H_j^{(n)}$ is bounded. This is why we decompose the unbounded Hamiltonians H_j into a sum of finite-dimensional operators $H_j^{(n)}$. Otherwise, the boundary triplet construction of Section 4.2.1 would fail.*

We can use Lemma 4.2.1 to obtain boundary triplets $\Pi_j^{(n)} = (\mathcal{H}_j^{(n)}, \Gamma_{0,j}^{(n)}, \Gamma_{1,j}^{(n)})$ with

$$\Gamma_{0,j}^{(n)} \vec{f}_j^{(n)} = y_j^{(n)}, \quad \Gamma_{1,j}^{(n)} \vec{f}_j^{(n)} = -P_{\mathcal{H}_j^{(n)}} f_j^{(n)}, \quad \vec{f}_j^{(n)} = (f_j^{(n)}, H_j^{(n)} f_j^{(n)} + y_j^{(n)}) \in (A_j^{(n)})^*.$$

The γ-field and the Weyl function are

$$\gamma_j^{(n)}(\zeta) = -(H_j^{(n)} - \zeta)^{-1} \restriction \mathcal{H}_j^{(n)} \quad \text{and} \quad M_j^{(n)}(\zeta) = P_{\mathcal{H}_j^{(n)}}(H_j^{(n)} - \zeta)^{-1} \restriction \mathcal{H}_j^{(n)}$$

for $\zeta \in \rho(H_j^{(n)})$. Also, $H_j^{(n)} = \ker(\Gamma_{0,j}^{(n)})$. We may take the direct sum

$$A^{(n)} = A_l^{(n)} \oplus A_S^{(n)} \oplus A_r^{(n)}$$

and obtain a boundary triplet

$$\widetilde{\Pi}^{(n)} = (\mathcal{H}^{(n)}, \widetilde{\Gamma}_0^{(n)}, \widetilde{\Gamma}_1^{(n)}) = \Pi_l^{(n)} \oplus \Pi_S^{(n)} \oplus \Pi_r^{(n)}$$

with Weyl function

$$\widetilde{M}^{(n)}(\zeta) = M_l^{(n)}(\zeta) \oplus M_S^{(n)}(\zeta) \oplus M_r^{(n)}(\zeta), \quad \zeta \in \rho(H_0).$$

It satisfies $\ker(\widetilde{\Gamma}_0^{(n)}) = H_0^{(n)}$, where

$$H_0^{(n)} = (h_l^{el} \oplus h_S^{el} \oplus h_r^{el}) \otimes I_{\mathbb{C}\Upsilon_n} + n\omega\, I_{el} \otimes I_{\mathbb{C}\Upsilon_n}.$$

We want to sum up these boundary triplets to obtain a boundary triplet for A^* given by

$$A = \bigoplus_{n \in \mathbb{N}_0} A^{(n)}.$$

To be able to do this, we apply Lemma 4.1.9 to transform $\widetilde{\Pi}^{(n)}$ into the boundary triplet $\Pi^{(n)} = (\mathcal{H}^{(n)}, \Gamma_0^{(n)}, \Gamma_1^{(n)})$ with Weyl function $M^{(n)}$ satisfying $M^{(n)}(i) = i$. We set

$$Q^{(n)} = \Re\mathrm{e}(\widetilde{M}^{(n)}(i)), \qquad R^{(n)} = \sqrt{\Im\mathrm{m}(\widetilde{M}^{(n)}(i))},$$

and define

$$\Gamma_0^{(n)} = R^{(n)}\widetilde{\Gamma}_0^{(n)}, \qquad \Gamma_1^{(n)} = (R^{(n)})^{-1}(\widetilde{\Gamma}_1^{(n)} - Q^{(n)}\widetilde{\Gamma}_0^{(n)}).$$

Note that still $\ker(\Gamma_0^{(n)}) = H_0^{(n)}$. By Theorem 4.1.11 the direct sum

$$\Pi = \bigoplus_{n \in \mathbb{N}_0} \Pi^{(n)} \tag{4.18}$$

is a boundary triplet for A^* and satisfies $\ker(\Gamma_0) = H_0$. Its boundary value space is $\mathcal{H} = \mathcal{H}_l \oplus \mathcal{H}_S \oplus \mathcal{H}_r$ with

$$\mathcal{H}_S = \bigoplus_{n \in \mathbb{N}_0} \mathfrak{h}_S^{el} \otimes \mathbb{C}\Upsilon_n = \mathfrak{h}_S^{el} \otimes \mathfrak{h}^{ph}, \qquad \mathcal{H}_j = \bigoplus_{n \in \mathbb{N}_0} \mathcal{H}_j^{el} \otimes \mathbb{C}\Upsilon_n = \mathcal{H}_j^{el} \otimes \mathfrak{h}^{ph},$$

for $j \in \{l, r\}$. This gives us $\mathcal{H} = (\mathcal{H}_l^{el} \oplus \mathfrak{h}_S^{el} \oplus \mathcal{H}_r^{el}) \otimes \mathfrak{h}^{ph}$. Now we have to find the correct extension parameter. For the coupling of the leads, recall the extension parameter $B^{el} = -(P_{\mathcal{H}^{el}}\tau_{el}v_{el} \restriction \mathcal{H}^{el})^{-1}$ defined in Lemma 4.2.3. Inspired by this, we define $\widetilde{B} = -(P_{\mathcal{H}}(\tau_{el}V_{el} + \tau_{int}V_{int}) \restriction \mathcal{H})^{-1}$. From the definition of V_{el} and V_{int}, it is

straightforward to check that

$$\mathrm{clo}\big(\mathrm{ran}(\tau_{el}V_{el} + \tau_{int}V_{int})\big) = \mathcal{H},$$

whence this inverse is well-defined. Furthermore, $V_{int} \restriction \mathcal{H}_S^{(n)}$ grows like $\sqrt{n}$ for large $n \in \mathbb{N}_0$, whence $\widetilde{B}$ is bounded. Obviously, this definition implies that the inverse of $\widetilde{B}$ is a densely defined self-adjoint operator with $\mathrm{dom}(H_0) \subset \mathrm{dom}(\widetilde{B}^{-1})$. We want to use the operator $\widetilde{B}$ as an extension parameter. However, we did transform the boundary triplets in order to be able to build the direct sum. We have to apply an according transformation to $\widetilde{B}$. For any bounded linear operator $\widetilde{X}^{(n)}$ on $\mathcal{H}^{(n)}$, we have

$$\widetilde{\Gamma}_1^{(n)} - \widetilde{X}^{(n)}\widetilde{\Gamma}_0^{(n)} = R^{(n)}\Gamma_1^{(n)} + Q^{(n)}(R^{(n)})^{-1}\Gamma_0^{(n)} - \widetilde{X}^{(n)}(R^{(n)})^{-1}\Gamma_0^{(n)}.$$

It follows that

$$\ker\Big(\widetilde{\Gamma}_1^{(n)} - \widetilde{X}^{(n)}\widetilde{\Gamma}_0^{(n)}\Big) = \ker\Big(\Gamma_1^{(n)} - (R^{(n)})^{-1}\big(\widetilde{X}^{(n)} - Q^{(n)}\big)(R^{(n)})^{-1}\Gamma_0^{(n)}\Big).$$

Thus, when transforming the boundary triplet, the extension parameter has to be transformed accordingly. Note, however, that V_{int} and hence $\widetilde{B}$ is not reduced by the spaces $\mathcal{H}^{(n)}$, $n \in \mathbb{N}_0$, whence we have to apply the corresponding transformation on the whole space $\mathcal{H}$ to $\widetilde{B}$. Define $\widetilde{B}_{nm} = P_{\mathcal{H}^{(n)}}\widetilde{B} \restriction \mathcal{H}^{(m)}$, $m, n \in \mathbb{N}_0$. Furthermore,

$$R = \bigoplus_{n\in\mathbb{N}_0} R^{(n)}, \qquad Q = \bigoplus_{n\in\mathbb{N}_0} Q^{(n)}.$$

Since $\|(H_j^{(n)} - i)^{-1}\| \leq \frac{c}{1+n}$ for some $c > 0$ independent of n, R and Q are bounded self-adjoint operators. Since $R^{(n)}$ is invertible for every $n \in \mathbb{N}_0$, the inverse R^{-1} is well-defined as an unbounded self-adjoint operator on $\mathrm{dom}(R^{-1}) = \mathrm{ran}(R)$. We define

$$B' = R^{-1}(\widetilde{B} - Q)R^{-1}, \quad \mathrm{dom}(B') = \Big\{\psi \in \mathcal{H} \,\Big|\, \psi, (\widetilde{B} - Q)R^{-1}\psi \in \mathrm{dom}(R^{-1})\Big\}. \quad (4.19)$$

Since $\widetilde{B}_{nm}^* = \widetilde{B}_{mn}$, $m, n \in \mathbb{N}_0$, we have

$$\begin{aligned}\langle\psi_1, B'\psi_2\rangle &= \sum_{m,n\in\mathbb{N}_0} \langle\psi_1^{(n)}, (R^{(n)})^{-1}\big(\widetilde{B}_{nm} - \delta_{nm}Q^{(m)}\big)(R^{(m)})^{-1}\psi_2^{(m)}\rangle \\ &= \sum_{m,n\in\mathbb{N}_0} \big\langle(R^{(m)})^{-1}\big(\widetilde{B}_{mn} - \delta_{mn}Q^{(n)}\big)(R^{(n)})^{-1}\psi_1^{(n)}, \psi_2^{(m)}\big\rangle.\end{aligned}$$

Thus, B' is symmetric and hence closable. We choose the extension parameter B to be the closure of B'. We still have to show that B is indeed the correct extension parameter. Furthermore, in order to fulfill the requirements of Theorem 4.1.14, we have to show that $(B + \theta)^{-1} \in \mathfrak{L}_1(\mathcal{H})$ for some $\theta > 0$.

Lemma 4.2.5. *The extension operator B satisfies $H = \ker(\Gamma_1 - B\Gamma_0)$, and $(B + \theta)^{-1}$ is trace class for some $\theta > 0$.*

Proof. Recall that

$$\widetilde{B} = -(P_{\mathcal{H}}(\tau_{el}V_{el} + \tau_{int}V_{int}) \restriction \mathcal{H})^{-1} = -\big(P_{\mathcal{H}}(H - H_0) \restriction \mathcal{H}\big)^{-1}.$$

Also,

$$A^* = \Big\{(f, H_0 f + y) \,\Big|\, \sum_{n\in\mathbb{N}_0} \|f^{(n)}\|^2 + \|H_0^{(n)} f^{(n)}\|^2 + \|y^{(n)}\|^2 < \infty\Big\}.$$

We have

$$\begin{aligned}
&\ker(\Gamma_1 - B\Gamma_0)\\
&\quad = \{\vec{f} \in A^* \,|\, \exists\, g \in \mathrm{dom}(B) \,:\, (\Gamma_0\vec{f}, \Gamma_1\vec{f}) = (g, Bg)\}\\
&\quad = \{\vec{f} \in A^* \,|\, \exists\, g \in \mathrm{dom}(B)\ \forall\, n \in \mathbb{N}_0 \,:\, (\Gamma_0^{(n)}\vec{f}^{(n)}, \Gamma_1^{(n)}\vec{f}^{(n)}) = (g^{(n)}, (Bg)^{(n)})\}.
\end{aligned}$$

Let $\vec{f} \in \ker(\Gamma_1 - B\Gamma_0)$ and $g \in \mathrm{dom}(B)$. Note that $(\Gamma_0^{(n)}\vec{f}^{(n)}, \Gamma_1^{(n)}\vec{f}^{(n)}) = (g^{(n)}, (Bg)^{(n)})$ is equivalent to

$$\begin{aligned}
&(R^{(n)}\widetilde{\Gamma}_0^{(n)}\vec{f}^{(n)}, (R^{(n)})^{-1}(\widetilde{\Gamma}_1^{(n)} - Q^{(n)}\widetilde{\Gamma}_0^{(n)})\vec{f}^{(n)})\\
&\quad = \Big(g^{(n)}, \sum_{m\in\mathbb{N}_0} (R^{(n)})^{-1}(\widetilde{B}_{nm} - \delta_{mn}Q^{(m)})(R^{(m)})^{-1}g^{(m)}\Big).
\end{aligned}$$

This implies

$$(\widetilde{\Gamma}_0^{(n)}\vec{f}^{(n)}, \widetilde{\Gamma}_1^{(n)}\vec{f}^{(n)}) = \Big(\widetilde{g}^{(n)}, \sum_{m\in\mathbb{N}_0} \widetilde{B}_{nm}\widetilde{g}^{(m)}\Big)$$

with $\widetilde{g}^{(n)} = (R^{(n)})^{-1}g^{(n)}$. From this we obtain

$$-P_{\mathcal{H}^{(n)}} f^{(n)} = \sum_{m\in\mathbb{N}_0} \widetilde{B}_{nm} y^{(m)} = (\widetilde{B}y)^{(n)},$$

i.e. $-P_{\mathcal{H}}f = \widetilde{B}y$. This in turn gives $y = -\widetilde{B}^{-1}f = (H - H_0)f$ since $f \in \ker(\Gamma_1 - B\Gamma_0)$ implies $f \in \mathrm{dom}(H) = \mathrm{dom}(H_0) \subset \mathrm{dom}(\widetilde{B}^{-1})$. Thus,

$$\vec{f} = \{(f^{(n)}, H_0^{(n)} f^{(n)} + y^{(n)})\}_{n\in\mathbb{N}_0} = (f, H_0 f + (H - H_0)f) = (f, Hf).$$

Since we know that B is closed and H is self-adjoint, it follows from 4.1.5 that B is self-adjoint. It remains to show that $(B + \theta)^{-1} \in \mathfrak{L}_1(\mathcal{H})$ for some $\theta > 0$. Since we already know that $H_0 = \ker(\Gamma_0)$ and $H = \ker(\Gamma_1 - B\Gamma_0)$, the Krein-type resolvent formula of Lemma 4.1.8 gives us

$$(H - \zeta_0)^{-1} = (H_0 - \zeta_0)^{-1} + \gamma(\zeta_0)\big(B - M(\zeta_0)\big)^{-1}\gamma(\overline{\zeta_0})^*$$

for $\zeta_0 \in \rho(H_0) \cap \rho(H))$. Since $\gamma(\zeta_0)$ is invertible, from $(H - \zeta_0)^{-1} - (H_0 - \zeta_0)^{-1} \in \mathfrak{L}_1(\mathfrak{H})$ it follows that $(B - M(\zeta_0))^{-1} \in \mathfrak{L}_1(\mathcal{H})$. The resolvent equation gives us

$$(B - i)^{-1} = \big(B - M(\zeta_0)\big)^{-1} + \big(B - M(\zeta_0)\big)^{-1}\big(M(\zeta_0) - i\big)(B - i)^{-1}.$$

Since B is self-adjoint, $(B - i)^{-1}$ is bounded. But $(B - M(\zeta_0))^{-1} \in \mathfrak{L}_1(\mathcal{H})$ and $M(\zeta_0)$

is bounded, whence $(B-i)^{-1} \in \mathfrak{L}_1(\mathcal{H})$. Since this implies that the discrete spectrum of B accumulates at most at infinity, we find some $\theta > 0$ satisfying $\theta \in \mathbb{R} \setminus \sigma(B)$. But then $(B+\theta)^{-1}$ is also trace class since $(B-i)^{-1} \in \mathfrak{L}_1(\mathcal{H})$ and

$$(B+\theta)^{-1} = (B-i)^{-1} - (i+\theta)(B-i)^{-1}(B+\theta)^{-1}.$$

□

Note that the proof shows that $(B+\theta)^{-1} \in \mathfrak{L}_1(\mathcal{H})$ for some $\theta > 0$ holds true in general if B is self-adjoint and the resolvent difference of H_0 and $H = \ker(\Gamma_1 - B\Gamma_0)$ is trace class. It follows that the boundary triplet $\Pi_\theta = (\mathcal{H}, \Gamma_0, \Gamma_1 + \theta\Gamma_0)$ that we obtain from the boundary triplet Π given by (4.18) and the extension parameter $B_\theta = B + \theta$ with B given by (4.19) satisfies the requirements of Theorem 4.1.14. Hence, we are able to explicitly calculate the transition matrix of the Jaynes-Cummings QD-LED.

Theorem 4.2.6. *The transition matrix of the Jaynes-Cummings QD-LED is given by*

$$T(\lambda) = -\pi^{-1}\,\Im\mathrm{m}\big(\widetilde{M}(\lambda)\big)^{\frac{1}{2}}\big(\widetilde{B} - \widetilde{M}(\lambda)\big)^{-1}\Im\mathrm{m}\big(\widetilde{M}(\lambda)\big)^{\frac{1}{2}}, \qquad \lambda \in \sigma(H_0), \tag{4.20}$$

where $\widetilde{M}(\lambda) = \bigoplus_{n\in\mathbb{N}_0} \widetilde{M}^{(n)}(\lambda)$ *and* $\mathrm{ran}\big(\Im\mathrm{m}\big(\widetilde{M}(\lambda)\big)^{\frac{1}{2}}\big)$ *is finite-dimensional.*

Proof. Let M_θ denote the Weyl function of Π_θ. Then Theorem 4.1.14 gives us

$$T(\lambda) = -\pi^{-1}\,\Im\mathrm{m}\big(M_{B_\theta}(\lambda)\big)^{\frac{1}{2}}\big(\mathrm{sgn}(B_\theta) - M_{B_\theta}(\lambda)\big)^{-1}\Im\mathrm{m}\big(M_{B_\theta}(\lambda)\big)^{\frac{1}{2}}, \qquad \lambda \in \sigma(H_0).$$

Recall that $M_{B_\theta}(\zeta) = |B_\theta|^{-\frac{1}{2}}\big(M(\zeta)+\theta\big)|B_\theta|^{-\frac{1}{2}}$, where $M(\zeta)$ is given by

$$M(\zeta) = \bigoplus_{n\in\mathbb{N}_0} (R^{(n)})^{-1}\big(\widetilde{M}^{(n)}(\zeta) - Q^{(n)}\big)(R^{(n)})^{-1}, \qquad \zeta \in \rho(H_0),$$

with

$$Q^{(n)} = \Re\mathrm{e}\big(\widetilde{M}^{(n)}(i)\big), \qquad R^{(n)} = \sqrt{\Im\mathrm{m}\big(\widetilde{M}^{(n)}(i)\big)}.$$

Since $Q^{(n)}$ is selfadjoint for $n \in \mathbb{N}$, we have $\Im\mathrm{m}(Q^{(n)}) = 0$. This implies

$$\Im\mathrm{m}\big(M(\zeta)\big) = \bigoplus_{n\in\mathbb{N}_0} (R^{(n)})^{-1}\Im\mathrm{m}\big(\widetilde{M}^{(n)}(\zeta)\big)(R^{(n)})^{-1}$$

Note that $\Im\mathrm{m}\big(\widetilde{M}_S^{(n)}(\lambda)\big) = 0$ for a.e. $\lambda \in \mathbb{R}$ since $\sigma(H_S) = \sigma_{pp}(H_S)$. The Weyl function in the leads is $\widetilde{M}_j^{(n)}(\zeta) = -P_{\mathcal{H}_j^{(n)}}(H_j^{(n)} - \zeta) \restriction \mathcal{H}_j^{(n)}$, $j \in \{l, r\}$, where $H_j^{(n)} = -\Delta^D + n\omega + v_j$ and we know the resolvent explicitly (cf. Lemma 3.2.2). Similarly to the electric model of the previous Section 4.2.1, we obtain

$$\widetilde{M}_j^{(n)}(\lambda) = \lim_{\epsilon\to+0}\int_{|\mu-\lambda|>\epsilon} \mathrm{d}\mu\,|g_j(1,\mu-n\omega)|^2(\mu-\lambda)^{-1} + i\pi\,|g_j(1,\lambda-n\omega)|^2, \quad j \in \{l,r\},$$

for $\lambda \in \mathbb{R}$. This implies that $\Im\mathrm{m}\big(\widetilde{M}_j^{(n)}(\lambda)\big) \neq 0$ only if $\frac{\lambda-v_j-4}{\omega} > n > \frac{\lambda-v_j}{\omega}$, whence $\Im\mathrm{m}\big(\widetilde{M}(\lambda)\big) = \bigoplus_{n\in\mathbb{N}_0}\Im\mathrm{m}\big(\widetilde{M}^{(n)}(\lambda)\big)$ is a well-defined finite-dimensional operator. It

follows that we can use the same scheme as in the proof of Corollary 4.1.15 to calculate

$$\Im\mathrm{m}\big(M_{B_\theta}(\lambda)\big)^{\frac{1}{2}} = U_\theta^*(\lambda)\Im\mathrm{m}\big(\widetilde{M}(\lambda)\big)^{\frac{1}{2}} R^{-1}|B_\theta|^{-\frac{1}{2}}.$$

Using $B_\theta = R^{-1}(\widetilde{B} - Q)R^{-1} + \theta$, we obtain

$$|B_\theta|^{-\frac{1}{2}}\big(\mathrm{sgn}(B_\theta) - M_{B_\theta}(\lambda)\big)^{-1}|B_\theta|^{-\frac{1}{2}} = R\big(\widetilde{B} - \widetilde{M}(\lambda)\big)^{-1}R,$$

whence

$$T(\lambda) = -\pi^{-1}\, U_\theta^*(\lambda)\Im\mathrm{m}\big(\widetilde{M}(\lambda)\big)^{\frac{1}{2}}\big(\widetilde{B} - \widetilde{M}(\lambda)\big)^{-1}\Im\mathrm{m}\big(\widetilde{M}(\lambda)\big)^{\frac{1}{2}} U_\theta(\lambda).$$

As in the proof of Corollary 4.1.15, we can eliminate $U_\theta(\lambda)$ with a suitably chosen spectral representation. Thus, the theorem follows. □

Note that the fact that $\mathcal{H}(\lambda)$ is finite-dimensional corresponds to $\dim(\mathfrak{h}(\lambda)) < \infty$, cf. Section 3.2. It remains to calculate $P_{\mathcal{H}(\lambda)}\big(B - M(\lambda)\big)^{-1} \restriction \mathcal{H}(\lambda)$ to know the transition matrix, whence Theorem 4.2.6 provides a starting point for the numerical computation of the matrix elements of the transition matrix.

4.2.3 An example for a Jaynes-Cummings quantum dot LED

Choose a two-level quantum dot with eigenvalues $\lambda_0 = 1$ and $\lambda_1 = 4$. Let the cavity be perfectly tuned, i.e. $\omega_0 = \omega = 3$. For $n \in \mathbb{N}_0$ we obtain

$$H_S^{(n)} = \begin{pmatrix} 1+3n & 0 \\ 0 & 4+3n \end{pmatrix}.$$

The Weyl function $\widetilde{M}_S^{(n)}(\lambda)$ is given by

$$\widetilde{M}_S^{(n)}(\lambda) = (H_S^{(n)} - \lambda)^{-1} = \begin{pmatrix} (1+3n-\lambda)^{-1} & 0 \\ 0 & (4+3n-\lambda)^{-1} \end{pmatrix}. \tag{4.21}$$

Choose the potentials of the leads as $v_l = 2$ and $v_r = 0$. This results in the spectrum

$$\sigma_{ac}(H_0) = \bigcup_{n\in\mathbb{N}_0} [3n, 6+3n] = \mathbb{R}_+.$$

The Weyl functions for the leads are

$$\widetilde{M}_j^{(n)}(\lambda) = \lim_{\epsilon\to+0}\int_{|\lambda-3n-\mu|>\epsilon} \mathrm{d}\mu\, |g_j(1,\mu)|^2(\mu+3n-\lambda)^{-1} + i\pi\, |g_j(1,\lambda-3n)|^2 \tag{4.22}$$

for $\lambda \in \sigma_{ac}(H_0)$, $n \in \mathbb{N}_0$, $j \in \{l, r\}$, where

$$g_l(1,\nu) = \pi^{-\frac{1}{2}}(1-(\nu-4)^2/4)^{\frac{1}{4}}, \qquad \nu \in (2,6),$$

and

$$g_r(1,\nu) = \pi^{-\frac{1}{2}}(1-(\nu-2)^2/4)^{\frac{1}{4}}, \qquad \nu \in (0,4).$$

Thus, $\Im\mathrm{m}(\widetilde{M}_l^{(n)}(\lambda)) = \pi|g_l(1,\lambda-3n)|^2 = 0$ if $\lambda - n\omega \notin (2,6)$ and $\Im\mathrm{m}(\widetilde{M}_r^{(n)}(\lambda)) = 0$ if $\lambda - n\omega \notin (0,4)$. This implies

$$\dim\Big(\mathrm{ran}\Big(\Im\mathrm{m}(\widetilde{M}^{(n)}(\lambda))\Big)\Big) = \begin{cases} 2 & \text{if } \lambda \in (2+3n, 4+3n), \\ 1 & \text{if } \lambda \in (3n, 2+3n) \cup (4+3n, 6+3n), \\ 0 & \text{if } \lambda \notin (3n, 6+3n). \end{cases}$$

Figure 4.1 shows a sketch of the absolutely continuous spectrum of H_0 and its multiplicity. Let $\widetilde{M}(\lambda) = \bigoplus_{n\in\mathbb{N}_0} \widetilde{M}^{(n)}(\lambda)$, where the sum is in fact finite. For $\lambda \in \mathbb{R}_+$ it follows that

$$\dim\Big(\mathrm{ran}\Big(\Im\mathrm{m}(\widetilde{M}(\lambda))\Big)\Big) = \begin{cases} 3 & \text{if } \exists\, n \in \mathbb{N}_0 : \lambda \in (2+3n, 4+3n),\ \lambda \geq 3 \\ 1 & \text{if } \lambda \in (0,2), \\ 2 & \text{otherwise.} \end{cases}$$

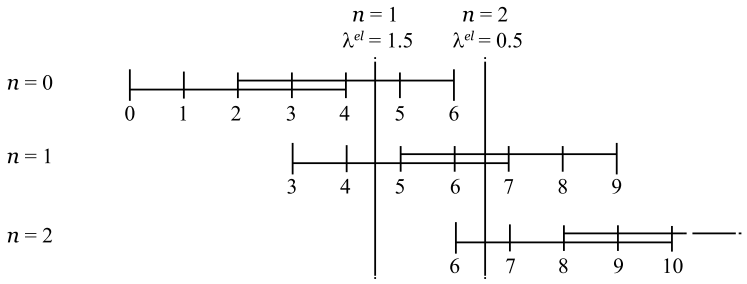

Figure 4.1: Absolutely continuous spectrum of the Jaynes-Cummings QD-LED

Fix $\lambda \in \mathbb{R}_+$. Let $n \in \mathbb{N}_0$ be the smallest number such that there is a $\lambda^{el} \in [0,3)$ with $\lambda = \lambda^{el} + 3n$, cf. Figure 4.1. Setting $\widetilde{M}_j^{(-1)}(\lambda) = 0$, we calculate

$$\Im\mathrm{m}(\widetilde{M}(\lambda)) = \begin{cases} \Im\mathrm{m}(\widetilde{M}_l^{(n-1)}(\lambda)) \oplus \Im\mathrm{m}(\widetilde{M}_r^{(n-1)}(\lambda)) \oplus \Im\mathrm{m}(\widetilde{M}_l^{(n)}(\lambda)) & \text{if } \lambda^{el} \in [0,1), \\ \Im\mathrm{m}(\widetilde{M}_r^{(n-1)}(\lambda)) \oplus \Im\mathrm{m}(\widetilde{M}_l^{(n)}(\lambda)) & \text{if } \lambda^{el} \in [1,2), \\ \Im\mathrm{m}(\widetilde{M}_r^{(n-1)}(\lambda)) \oplus \Im\mathrm{m}(\widetilde{M}_l^{(n)}(\lambda)) \oplus \Im\mathrm{m}(\widetilde{M}_r^{(n)}(\lambda)) & \text{if } \lambda^{el} \in [2,3). \end{cases}$$

According to Theorem 4.2.6, the transition matrix is given by.

$$T(\lambda) = -\pi^{-1}\Im\mathrm{m}(\widetilde{M}(\lambda))^{\frac{1}{2}}(\widetilde{B} - \widetilde{M}(\lambda))^{-1}\Im\mathrm{m}(\widetilde{M}(\lambda))^{\frac{1}{2}}$$

We calculated $\Im\mathrm{m}(\widetilde{M}(\lambda))^{\frac{1}{2}}$, so it remains to compute $P_{\widetilde{\mathcal{H}}(\lambda)}(\widetilde{B} - \widetilde{M}(\lambda))^{-1} \restriction \widetilde{\mathcal{H}}(\lambda)$, where $\widetilde{\mathcal{H}}(\lambda) = \mathrm{ran}(\Im\mathrm{m}(\widetilde{M}(\lambda))^{\frac{1}{2}})$. Since in general $\widetilde{B}$ mixes all channels n in the decomposition $\widetilde{M}(\lambda) = \bigoplus_{n\in\mathbb{N}_0} \widetilde{M}^{(n)}(\lambda)$ due to the electron-photon interaction term V_{int}, we do not get a more explicit analytic expression for the transition matrix than this. However, if one wants to do numerical computations, one can use the fact that $\widetilde{M}^{(m)}(\lambda)$ decays in m. Namely, if we fix $\lambda = \lambda^{el} + 3n$, we see from (4.21) and (4.22) that $\widetilde{M}^{(m)}(\lambda)$ decays as $|m-n|$ grows. Hence, for numerical calculations one can use that $\widetilde{B}^{-1}$ is known

explicitly to write

$$\big(\widetilde{B} - \widetilde{M}(\lambda)\big)^{-1} = \widetilde{B}^{-1}\big(1 - \widetilde{M}(\lambda)\widetilde{B}^{-1}\big)^{-1},$$

an then assume that $1 - \widetilde{M}(\lambda)\widetilde{B}^{-1} \restriction \operatorname{ran}(\Im\mathrm{m}(\widetilde{M}^{(n)}(\lambda))) = 1$ for $m \in \mathbb{N}$ such that $|m-n|$ sufficiently large. Then the calculation of $(\widetilde{B} - \widetilde{M}(\lambda))^{-1}$ reduces to solving a finite system of linear equations.

For a certain choice of the coupling, we can even calculate $(\widetilde{B} - \widetilde{M}(\lambda))^{-1}$ analyticly. Namely, if we choose the coupling of the leads such that the left lead couples to the excited state and the right leads couples to the ground state of the quantum dot, i.e. $x_S^0 = e_1$ and $x_S^1 = e_0$ (cf. Figure 4.2), the extension parameter $\widetilde{B}$ and the Weyl function $\widetilde{M}(\lambda)$ are simultaneously reduced by a decomposition of $\mathcal{H}$. This coupling actually implies that the coupling-induced electric current is zero, since we can consider $\mathfrak{h}_l^{el} \oplus \mathbb{C}e_1$ and $\mathbb{C}e_0 \oplus \mathfrak{h}_r^{el}$ as two independent subsystems, and the only possibility for an electron to travel from left to right is to drop from the excited state e_1 to the ground state e_0 by emitting a photon.

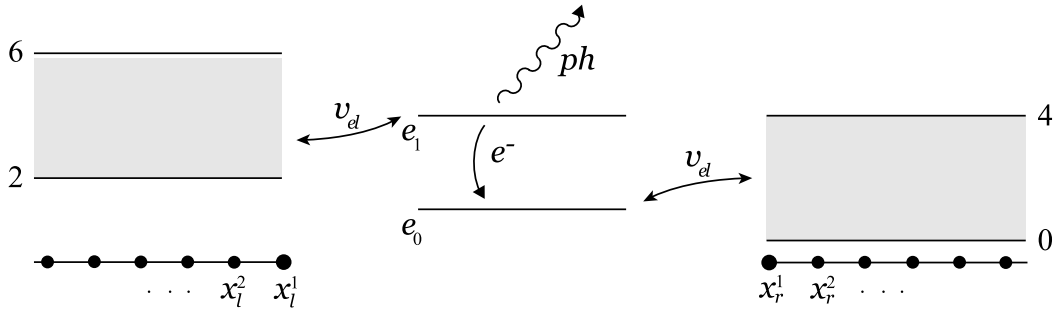

Figure 4.2: 2-level Jaynes-Cummings QD-LED with coupling to energy levels

For $n \in \mathbb{N}$, consider the subspaces $\mathcal{H}_S^{(n)} = \mathfrak{H}_S^{(n)} = \operatorname{span}\{e_0 \otimes \Upsilon_n, e_1 \otimes \Upsilon_{n-1}\}$. We define

$$\mathfrak{K}^{(n)} = \mathcal{H}_l^{(n-1)} \oplus \Big(\mathbb{C}(e_1 \otimes \Upsilon_{n-1}) \oplus \mathbb{C}(e_0 \otimes \Upsilon_n)\Big) \oplus \mathcal{H}_r^{(n)}, \quad \mathfrak{K}^{(0)} = \mathbb{C}(e_0 \otimes \Upsilon_0) \oplus \mathcal{H}_r^{(0)}.$$

Then $\mathcal{H} = \bigoplus_{n\in\mathbb{N}_0} \mathfrak{K}^{(n)}$. With respect to this decomposition, we have $\widetilde{B} = \bigoplus_{n\in\mathbb{N}_0} \widetilde{B}_n$, where $\widetilde{B}_n$ is given by

$$\widetilde{B}_n = \begin{pmatrix} 0 & \tau_{el} & 0 & 0 \\ \tau_{el} & 0 & \tau_{int}\sqrt{n} & 0 \\ 0 & \tau_{int}\sqrt{n} & 0 & \tau_{el} \\ 0 & 0 & \tau_{el} & 0 \end{pmatrix}^{-1}, \qquad \widetilde{B}_0 = \begin{pmatrix} 0 & \tau_{el} \\ \tau_{el} & 0 \end{pmatrix}^{-1}, \qquad n \in \mathbb{N}.$$

The Weyl function decomposes into $\widetilde{M}(\lambda) = \bigoplus_{n\in\mathbb{N}_0} \widetilde{M}_n(\lambda)$, where for $n \in \mathbb{N}$

$$\widetilde{M}_n(\lambda) = \widetilde{M}_l^{(n-1)}(\lambda) \oplus \widetilde{M}_{S,n}(\lambda) \oplus \widetilde{M}_r^{(n)}(\lambda), \qquad \widetilde{M}_0(\lambda) = \widetilde{M}_S^{(0)}(\lambda) \oplus M_r^{(0)}(\lambda)$$

and

$$\widetilde{M}_{S,n}(\lambda) = \begin{pmatrix} (1+3n-\lambda)^{-1} & 0 \\ 0 & (4+3(n-1)-\lambda)^{-1} \end{pmatrix}, \qquad M_{S,0}(\lambda) = (1-\lambda)^{-1}.$$

Thus, the calculation of $\left(\widetilde{B} - \widetilde{M}(\lambda)\right)^{-1}$ is nothing but the calculation of the inverse of the 4×4-matrix $\widetilde{B}_n - \widetilde{M}_n(\lambda)$ for every $n \in \mathbb{N}_0$.

We refrain from further analytical or numerical analysis of the transition matrix and its implications on the Landauer-Büttiker formula. Although this is a very interesting aspect that deserves further attention, it would lead us beyond the scope of this thesis. However, we point out that the above analysis shows that the formula of Theorem 4.2.6 is an important step in the calculation of the transition matrix $T(\lambda)$ for the Jaynes-Cummings QD-LED. It shows that the formulae for the electric current and the photon production rate from Section 3.2 can actually be used to explicitly calculate these quantities.

5 A quantum dot LED based on a Pauli-Fierz model

In Chapter 3 we derived an abstract Landauer-Büttiker formula and applied it to a model of a QD-LED that is based on the Jaynes-Cummings model. The appeal of this model is that its simple structure gives us rich information on the spectrum of the Hamiltonians. Also, the trace class condition $(H-i)^{-1}-(H_0-i)^{-1}\in\mathfrak{L}_1(\mathfrak{H})$ is satisfied, which is a necessary condition for the Landauer-Büttiker formula of Theorem 3.1.2. The downside is that the model allows only photons of a single fixed frequency. In this chapter we want to get rid of this restriction by introducing a model with photons of arbitrary energy that is based on the 1-photon Pauli-Fierz model of Section 2.2 (see also [46, 50]). In this case the resolvent difference is no longer trace class, whence the Landauer-Büttiker formula of Chapter 3 does not apply. This forces us to prove an extension of the Landauer-Büttiker formula. The main idea is to formulate the problem in terms of a decoupled Hamiltonian that is a multiplication operator $\mathcal{M}(H_0(\mu))$ on $L^2(\mathbb{R}^0_+,\mathrm{d}\mathfrak{m}(\mu),\mathfrak{h})$. Then the coupling of the leads is also a multiplication operator that is relatively trace class in the fiber. Since the electron-photon interaction is relatively trace class on the whole space, it turns out that this is sufficient to prove a Landauer-Büttiker formula. In this setting the Landauer-Büttiker formula again gives us formulae for the electric current and the photon production rate.

The techniques we use for the proof are very similar to those used in Chapter 3, but the complexity of the model makes the proof of the Landauer-Büttiker formula much more involved. As before, we use Lemma 3.1.4 to obtain a spectral representation of $K_{0,ac}=\mathcal{M}(K_0^{ac}(\mu))$, but now the lemma gives us only a spectral representation of $K_0^{ac}(\mu)$ on the fiber that we have to raise to the full space. The proof also uses the stationary wave operators in the operator spectral integral representation, but difficulties arise in the existence of the limit of the resolvent towards the real axis. The important notion that resolves this issue is that of smoothness, which is a concept that carries over from the fiber to the full space, unlike the Hilbert-Schmidt property, which we used to obtain the existence of the limit in Proposition 3.1.6.

5.1 A Landauer-Büttiker formula for multiplication operators

In this section we present a Landauer-Büttiker formula for a certain class of multiplication operators. Before we begin with the definition of the abstract model, we motivate it with the example of the 1-photon Pauli-Fierz QD-LED. A detailed presentation of this model follows in Section 5.3. Recall from Section 2.2 that the photon Hamiltonian

of the 1-photon Pauli-Fierz model is given by

$$h^{ph} = \begin{pmatrix} 0 & 0 \\ 0 & \mathcal{M}(\omega(k)) \end{pmatrix},$$

whence a spectral representation on $L^2(\mathbb{R}^0_+, \mathrm{d}\mathfrak{m}(\mu), \mathbb{C}^2)$ with $\mathrm{d}\mathfrak{m}(\mu) = \mathrm{d}\mu + \delta(\mu)\mathrm{d}\mu$ is given by

$$(\phi^{ph}(f_0^{ph}, f_1^{ph}))(0) = (f_0^{ph}, 0), \qquad (\phi^{ph}(f_0^{ph}, f_1^{ph}))(\mu) = (f_1^{ph}(\mu), f_1^{ph}(-\mu)), \qquad \mu > 0.$$

In the 1-photon Pauli-Fierz QD-LED model, the decoupled Hamiltonian is given by $H_0 = h_0^{el} \otimes I_{ph} + I_{el} \otimes h^{ph}$, where h_0^{el} is some initial Hamiltonian for the electron system with decoupled leads. We can use the spectral representation ϕ^{ph} of h^{ph} to write

$$H_0 = \mathcal{M}(H_0(\mu)), \qquad H_0(\mu) = \begin{pmatrix} h_0^{el} + \mu & 0 \\ 0 & h_0^{el} + \mu \end{pmatrix}.$$

as multiplication operator on $L^2(\mathbb{R}^0_+, \mathrm{d}\mathfrak{m}(\mu), \mathfrak{h})$, where $\mathfrak{h} = \mathfrak{h}^{el} \otimes \mathbb{C}^2$. Similarly, we can write $H_{el} = h^{el} \otimes I_{ph} + I_{el} \otimes h^{ph} = \mathcal{M}\big(H_{el}(\mu)\big)$ for some coupled electron Hamiltonian h^{el}. The final Hamiltonian H_{ph} with the electron-photon interaction mixes the fibers and can not be written as a multiplication operator on the same space.

It turns out that $(H_{el} + i)^{-1} - (H_{ph} + i)^{-1}$ is trace class. If the resolvent difference $(h_0^{el}+i)^{-1} - (h^{el}+i)^{-1}$ is trace class, the resolvent difference $(H_0(\mu)+i)^{-1} - (H_{el}(\mu)-i)^{-1}$ in the fiber is also trace class for every $\mu \in \mathbb{R}^0_+$. However, since the measure $\mathfrak{m}$ has an absolutely continuous part, the total resolvent difference $(H_0 + i)^{-1} - (H_{el} + i)^{-1}$ is not trace class. This is the background that motivates us to develop an abstract Landauer-Büttiker formula for certain multiplication operators that goes beyond the trace class setting of Section 3.1.

5.1.1 The abstract model

Let $\mathfrak{H} = L^2(\mathbb{R}^0_+, \mathrm{d}\mathfrak{m}(\mu), \mathfrak{h})$, where $\mathrm{d}\mathfrak{m}(\mu) = \mathrm{d}\mu + \delta(\mu)\mathrm{d}\mu$. Let h_j be positive densely-defined self-adjoint operators with domain $\mathrm{dom}(h_j)$, $j \in \{0, 1\}$. Assume $\sigma(h_1) = \sigma_{ac}(h_1)$. Define $H_j = \mathcal{M}\big(H_j(\mu)\big)$, where $H_j(\mu) = h_j + \mu$. The domain of H_j is given by

$$\mathrm{dom}(H_j) = \Big\{ f \in \mathfrak{H} \,\Big|\, f(\mu) \in \mathrm{dom}(h_j)\ \mathfrak{m}\text{-a.e.}, \int_0^\infty \mathrm{d}\mathfrak{m}(\mu)\, \|\mu\, f(\mu)\|^2 < \infty \Big\}. \tag{A0}$$

Let further H_2 be densely-defined, self-adjoint, and positive on $\mathrm{dom}(H_2) \subset \mathfrak{H}$. Assume that

$$v_1 = c_1 z_1 c_1 = (h_0 + 1)^{-1} - (h_1 + 1)^{-1} \in \mathfrak{L}_1(\mathfrak{h}), \tag{A1}$$

where $c_1 = \sqrt{|v_1|} \in \mathfrak{L}_2(\mathfrak{h})$ and $z_1 = \mathrm{sgn}(v_1) \in \mathfrak{B}(\mathfrak{h})$, and

$$V_2 = C_2 Z_2 C_2 = (H_1 + 1)^{-1} - (H_2 + 1)^{-1} \in \mathfrak{L}_1(\mathfrak{H}), \tag{A2}$$

where $C_2 = \sqrt{|V_2|} \in \mathfrak{L}_2(\mathfrak{H})$ and $Z_2 = \mathrm{sgn}(V_2) \in \mathfrak{B}(\mathfrak{H})$ are self-adjoint.

Remark 5.1.1. *Obviously, the positivity is not essential since any operator that is bounded from below can be shifted to meet the requirements. Similarly, all the calculations of this section hold also for the more general space* $L^2(\mathbb{R}, \mathrm{d}\widetilde{\mathfrak{m}}(\mu), \mathfrak{h})$*, where the measure is given by*

$$\mathrm{d}\widetilde{\mathfrak{m}}(\mu) = \chi_\Xi(\mu)\mathrm{d}\mu + \sum_{n=1}^{N} \delta(\mu - \mu_n)\mathrm{d}\mu$$

for some bounded from below $\Xi \subset \mathbb{R}$ *and* $\mu_n \in \mathbb{R}$*,* $N \in \mathbb{N}$*. In particular,* $\Xi = \emptyset$ *and* $N = 1$ *with* $\mu_1 = 0$ *gives us the setting of the usual Landauer-Büttiker formula. In this sense, the new Landauer-Büttiker formula of Theorem 5.1.8 generalizes the formula of Theorem 3.1.2.*

The assumption that h_1 *is absolutely continuous is necessary for the unitarity of the scattering matrix. One obtains a Landauer-Büttiker formula without this unitarity, but it is needed to put it in the usual form.*

In the following we use lowercase letters for objects associated with h_j, $j \in \{0, 1\}$, e.g. $p^{ac}_{h_0}$ for the projection onto the absolutely continuous subspace of h_0. In contrast, we use uppercase letters for objects associated with H_j and $H_j(\mu)$, $j \in \{0, 1, 2\}$, $\mu \geq 0$, e.g. $P^{ac}_{H_0(\mu)}$ for the projection onto the absolutely continuous subspace of $H_0(\mu)$. Incidentally, we have $P^{ac}_{H_0(\mu)} = p^{ac}_{h_0}$. We define

$$V_1(\mu) = (h_0 + \mu + 1)^{-1} - (h_1 + \mu + 1)^{-1}$$

for $\mu \geq 0$ and

$$V_1 = \mathcal{M}\big(V_1(\mu)\big) = (H_0 + 1)^{-1} - (H_1 + 1)^{-1}.$$

Furthermore, we choose an initial state ρ that satisfies

$$\rho = \mathcal{M}\big(\rho_0\, \delta(\mu)\big), \qquad [\rho_0, h_0] = 0, \qquad \varrho_0 = \rho(H_0 + 1)^2 \in \mathfrak{B}(\mathfrak{H}). \tag{A3}$$

Just as in Chapter 3, a physical state ρ_0 should be positive and satisfy $\rho_0 \leq 1$. But this is not relevant for the mathematics, and thus we do not take it as a part of the assumptions. We assume that the observable Q for which we calculate the flux satisfies

$$Q = \mathcal{M}(q(\mu)) \in \mathfrak{B}(\mathfrak{H}), \quad [q(\mu), h_0] = 0, \quad q(\mu)p^{ac}_{h_0} = q(\mu), \quad \text{for } \mathfrak{m}\text{-a.e. } \mu \geq 0. \tag{A4}$$

Remark 5.1.2. *The restriction of the initial state to the fiber* $\mu = 0$ *is necessary to obtain well-defined traces in the Landauer-Büttiker formula. However, it is motivated by the initial state*

$$\rho = \rho_0^{el} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}.$$

in the 1-photon Pauli-Fierz QD-LED. This state corresponds to total darkness, i.e. initially no photons are present, which is the same as a photon field with temperature absolute zero. This is a natural starting point for the analysis of an LED.

Remark 5.1.3. *In the 1-photon Pauli-Fierz QD-LED, the two most important cases for the observable* Q *are* $p_j^{el} \otimes I_{ph}$*,* $j \in \{l, r\}$*, for the electron current and the photon number* $I_{el} \otimes \big(0 \oplus I_{\mathfrak{h}_1^{ph}}\big)$ *for the photon production rate. Their tensor product structure allows*

us to write them as multiplication operators of the above form. It is straightforward to generalize the model to unbounded observables as in the Landauer-Büttiker formula of Theorem 3.1.2. As the presentation is already rather complex, we use a bounded Q for more clarity.

The following decomposition of V_1 is used in the construction of a spectral representation of H_0^{ac} similar to that of Section 3.1. The crucial aspect in this decomposition is that $c_1 \in \mathfrak{L}_2(\mathfrak{h})$ and thus $C_1(\mu) = c_1 D_1(\mu)$ is Hilbert-Schmidt 'uniformly' in $\mu \geq 0$. We need this to raise the smoothness from the fiber to the whole space, cf. Section 5.2.1.

Lemma 5.1.4. *The resolvent difference $V_1 = (H_0+1)^{-1} - (H_1+1)^{-1}$ can be written as $V_1 = C_1^* Z_1 C_1$, where $C_1 = \mathcal{M}(C_1(\mu)) \in \mathfrak{B}(\mathfrak{H})$ and $Z_1 = \mathcal{M}(Z_1(\mu)) \in \mathfrak{B}(\mathfrak{H})$ with*

$$C_1(\mu) = c_1 D_1(\mu) \in \mathfrak{L}_2(\mathfrak{h}), \qquad Z_1(\mu) = z_1 - \mu\, z_1 c_1 D_0(\mu) c_1 z_1 \in \mathfrak{B}(\mathfrak{h}),$$

for $D_j(\mu) = (h_j+1)(h_j+\mu+1)^{-1}$, $j \in \{0,1\}$, for $\mathfrak{m}$-a.e. $\mu \geq 0$.

Proof. For $\mathfrak{m}$-a.e. $\mu \geq 0$, we have

$$\begin{aligned}
&(h_0+\mu+1)^{-1} - (h_1+\mu+1)^{-1} \\
&\quad = (h_1+\mu+1)^{-1}(h_1+1)\big((h_0+1)^{-1} - (h_1+1)^{-1}\big)(h_0+1)(h_0+\mu+1)^{-1} \\
&\quad = D_1(\mu) c_1 z_1 c_1 D_0(\mu),
\end{aligned}$$

where $c_1 \in \mathfrak{L}_2(\mathfrak{h})$ by Assumption (A1). Since

$$D_0(\mu) - D_1(\mu) = D_0(\mu)\big((h_1+\mu+1)(h_1+1)^{-1} - (h_0+\mu+1)(h_0+1)^{-1}\big) D_1(\mu)$$

and

$$(h_1+\mu+1)(h_1+1)^{-1} - (h_0+\mu+1)(h_0+1)^{-1} = \mu\big((h_1+1)^{-1} - (h_0+1)^{-1}\big) = -\mu\, c_1 z_1 c_1,$$

we obtain

$$(h_0+\mu+1)^{-1} - (h_1+\mu+1)^{-1} = D_1(\mu) c_1 \big(z_1 - \mu\, z_1 c_1 D_0(\mu) c_1 z_1\big) c_1 D_1(\mu).$$

□

5.1.2 The abstract Landauer-Büttiker formula

Just as in Chapter 3, we need the wave operators to define the steady state flux of the observable Q. Since the wave operators $W_\pm(H_1, H_0)$ do not exist on the whole space $\mathfrak{H}_{H_0}^{ac}$, we introduce $\mathfrak{H}_0^{ac} = \mathrm{ran}(P_0^{ac})$, with $P_0^{ac} = \mathcal{M}(p_{h_0}^{ac})$. We have $\mathfrak{H}_0^{ac} \subset \mathfrak{H}_{H_0}^{ac}$ since

$$P_{H_0}^{ac} = \mathcal{M}\big(P_{H_0}^{ac}(\mu)\big), \qquad P_{H_0}^{ac}(\mu) = \begin{cases} p_{h_0}^{ac} & \text{if } \mu = 0, \\ I_{\mathfrak{h}} & \text{if } \mu > 0. \end{cases}$$

Furthermore, since h_1 is absolutely continuous, we obtain $P_{H_1}^{ac} = \mathcal{M}(p_{h_1}^{ac}) = I_{\mathfrak{H}}$. Note that $\mathcal{M}(p_{h_1}^{ac})$ does not contain the independent variable μ since $p_{h_1}^{ac}$ is independent of μ.

We will encounter more such operators in this chapter. We write them as multiplication operators so one can easily see on which space the operators are acting.

Proposition 5.1.5. *The wave operators*

$$W_\pm(H_2, H_0) = W_\pm(H_2, H_1)W_\pm(H_1, H_0) = \operatorname*{s-lim}_{t\to\pm\infty} e^{itH_2}e^{-itH_0}P_0^{ac}$$

exist and are isometries on $\mathfrak{H}_0^{ac}$, where

$$W_\pm(H_1, H_0) = \operatorname*{s-lim}_{t\to\pm\infty} e^{itH_1}e^{-itH_0}P_0^{ac} = \mathcal{M}(W_\pm(h_1, h_0))$$

and

$$W_\pm(H_2, H_1) = \operatorname*{s-lim}_{t\to\pm\infty} e^{itH_2}e^{-itH_1}.$$

Furthermore, the scattering operator $S = W_+^*(H_2, H_0)W_-(H_2, H_0)$ is unitary on $\mathfrak{H}_0^{ac}$.

Proof. We have

$$e^{itH_1}e^{-itH_0}P_0^{ac} = \mathcal{M}(e^{ith_1}e^{-ith_0}p_{h_0}^{ac}),$$

whence

$$\begin{aligned} W_\pm(H_1, H_0) &= \operatorname*{s-lim}_{t\to\pm\infty} e^{itH_1}e^{-itH_0}P_0^{ac} \\ &= \operatorname*{s-lim}_{t\to\pm\infty} \mathcal{M}(e^{ith_1}e^{-ith_0}p_{h_0}^{ac}) \\ &= \mathcal{M}(W_\pm(h_1, h_0)), \end{aligned}$$

where $W_\pm(h_1, h_0)$ exist and are complete since $(h_1 + 1)^{-1} - (h_0 + 1)^{-1} \in \mathfrak{L}_1(\mathfrak{h})$ by Assumption (A1). Hence, $W_\pm(h_1, h_0)$ are isometries, which implies that $W_\pm(H_1, H_0)$ are isometries. Also, $(H_2 + 1)^{-1} - (H_1 + 1)^{-1} \in \mathfrak{L}_1(\mathfrak{H})$ by Assumption (A2), which implies that $W_\pm(H_2, H_1)$ exist and are complete. The chain rule for wave operators gives us that

$$W_\pm(H_2, H_0) = W_\pm(H_2, H_1)W_\pm(H_1, H_0)$$

exist and are isometries on $\mathfrak{H}_0^{ac}$. Let $S_2 = W_+^*(H_2, H_1)W_-(H_2, H_1)$. Since

$$W_\pm(H_1, H_0)W_\pm^*(H_1, H_0) = \mathcal{M}(p_{h_1}^{ac}) = I_{\mathfrak{H}}$$

and S_2 is unitary, we have

$$\begin{aligned} S^*S &= W_-^*(H_1, H_0)S_2^*W_+(H_1, H_0)W_+^*(H_1, H_0)S_2W_-(H_1, H_0) \\ &= W_-^*(H_1, H_0)W_-(H_1, H_0) \\ &= P_0^{ac}. \end{aligned}$$

□

In particular, the unitarity of S gives us the so-called optical theorem

$$T^* - T = 2\pi i\, T^*T,$$

cf. Lemma A.2.7. Since P_0^{ac} is not the whole absolutely continuous subspace of H_0, we have to give some thought to the steady state with respect to which we have to calculate

the current.

Proposition 5.1.6. *Let $\rho \in \mathfrak{B}(\mathfrak{H})$ be given by* (A3)*. If $\sigma_{sc}(H_2) = \emptyset$, the steady state*

$$\langle g, \rho_\infty f\rangle = \lim_{T\to+\infty} \frac{1}{T}\int_0^T \mathrm{d}t\, \langle g, e^{-itH_2}\rho\, e^{itH_2} f\rangle, \qquad f, g \in \mathfrak{H},$$

is given by the density operator

$$\rho_\infty = W_-(H_2, H_0)\rho\, W_-^*(H_2, H_0) + \rho_2^{pp}, \tag{5.1}$$

where

$$\rho_2^{pp} = \sum_{\lambda\in\sigma_{pp}(H_2)} E_{H_2}^{pp}(\{\lambda\})\rho E_{H_2}^{pp}(\{\lambda\}).$$

Proof. The proof is similar to the proof of [2, Thm. 3.2]. By [9, Cor. 14, Lemma 15], we may also use the weak, and thus in particular the strong limit of $e^{itH_2}\rho\, e^{-itH_2}$ if it exists. We have $\sigma_{sc}(H_2) = \emptyset$ by assumption. Hence,

$$e^{-itH_2}\rho\, e^{itH_2} = \sum_{j,m\in\{ac,pp\}} P_{H_2}^j e^{-itH_2}\rho\, e^{itH_2} P_{H_2}^m.$$

Note that $P_{H_2}^{pp} = \text{s-lim}_{n\to\infty} P^{(n)}$ for some family $\{P^{(n)}\}_{n\in\mathbb{N}}$ of finite rank orthogonal projections commuting with H_2. For $f \in \mathfrak{H}$ we have

$$\|P_{H_2}^{pp} e^{-itH_2}\rho\, e^{itH_2} P_{H_2}^{ac} f\| \le \|(P_{H_2}^{pp} - P^{(n)})\rho\, e^{itH_2^{ac}} f\| + \|P^{(n)}\rho\, e^{itH_2^{ac}} f\|.$$

We can make the first summand arbitrarily small by choosing $n \in \mathbb{N}$ large enough. Then we can choose $t \in \mathbb{R}$ large enough to make the second summand arbitrarily small using the Riemann-Lebesgue Lemma. We obtain $\lim_{t\to+\infty} \|P_{H_2}^{pp} e^{-itH_2}\rho\, e^{itH_2} P_{H_2}^{ac} f\| = 0$. It follows immediately that $\text{w-lim}_{t\to+\infty} P_{H_2}^{ac} e^{-itH_2}\rho\, e^{itH_2} P_{H_2}^{pp} = 0$ for the adjoint. For $f, g \in \mathfrak{H}$ the pure point part gives

$$\begin{aligned}
&\lim_{T\to+\infty} \frac{1}{T}\int_0^T \mathrm{d}t\, \langle g, e^{-itH_2^{pp}}\rho\, e^{itH_2^{pp}} f\rangle \\
&\quad= \sum_{\lambda,\nu\in\sigma_{pp}(H_2)} \lim_{T\to+\infty} \frac{1}{T}\int_0^T \mathrm{d}t\, e^{-it(\lambda-\nu)} \langle g, E_{H_2}^{pp}(\{\lambda\})\rho E_{H_2}^{pp}(\{\nu\}) f\rangle \\
&\quad= \left\langle g, \sum_{\lambda\in\sigma_{pp}(H_2)} E_{H_2}^{pp}(\{\lambda\})\rho E_{H_2}^{pp}(\{\lambda\}) f \right\rangle,
\end{aligned}$$

which gives us the second summand in (5.1). Since $W_-(H_2, H_1)$ is complete,

$$\begin{aligned}
&\text{w-}\lim_{t\to+\infty} P_{H_2}^{ac} e^{-itH_2}\rho\, e^{itH_2} P_{H_2}^{ac} \\
&\quad= \text{w-}\lim_{t\to+\infty} W_-(H_2, H_1) e^{-itH_1}\rho\, e^{itH_1} W_-^*(H_2, H_1)
\end{aligned} \tag{5.2}$$

Note that $\rho(\mu) = \delta(\mu)\rho_0$ for $\mathfrak{m}$-a.e. $\mu \geq 0$, whence

$$e^{-itH_1}\rho\, e^{itH_1} = \mathcal{M}\Big(p_{h_1}^{ac} e^{-ith_1}\rho_0 e^{ith_1} p_{h_1}^{ac}\delta(\mu)\Big).$$

Since $W_-(H_1, H_0) = \mathcal{M}\big(W_-(h_1, h_0)\big)$ and $[\rho_0, h_0] = 0$, we obtain

$$\begin{aligned}&\operatorname*{w-lim}_{t\to+\infty} W_-(H_2, H_1)e^{-itH_1}\rho\, e^{itH_1}W_-^*(H_2, H_1)\\ &\quad = W_-(H_2, H_1)W_-(H_1, H_0)\rho\, W_-^*(H_1, H_0)W_-^*(H_2, H_1).\end{aligned}$$

□

We already noted in Section 3.1 that the pure point part ρ_2^{pp} does not contribute to the flux. We are left with the following formal definition of the flux $\mathfrak{J}_Q$ of Q.

$$\mathfrak{J}_Q = i\,\mathrm{Tr}(W_-(H_2, H_0)\rho\, W_-^*(H_2, H_0)[H_2, Q]). \tag{5.3}$$

Just as in the case of the usual Landauer-Büttiker formula of Chapter 3, we use the invariance principle for wave operators to obtain a rigorous definition. We define

$$K_j = \varphi(H_j) = -(H_j + 1)^{-1}, \qquad j \in \{0, 1, 2\},$$

where $\varphi(\lambda) = -(\lambda + 1)^{-1}$ for $\lambda \geq 0$. From the invariance principle for the absolute Abelian limit, cf. Theorem A.2.13 in the appendix, we obtain

$$W_{1,\pm} = \operatorname*{|A|-lim}_{t\to\pm\infty} e^{itK_1}e^{-itK_0}P_0^{ac} = W_\pm(H_1, H_0) = \mathcal{M}(w_{1,\pm}),$$

where $w_{1,\pm} = W_\pm(k_1, k_0)$ with $k_1 = -(h_1 + 1)^{-1}$ and $k_0 = -(h_0 + 1)^{-1}$. The invariance principle for strong limits gives us

$$W_{2,\pm} = \operatorname*{s-lim}_{t\to\pm\infty} e^{itK_2}e^{-itK_1} = W_\pm(H_2, H_1).$$

Recall that we used certain sets $\Lambda_n \subset (-n, n)$, $n \in \mathbb{N}$, in the proof of Propostion 3.1.10 to obtain convergence uniform in λ of $C(H - \lambda \pm i\epsilon)^{-1}C$ as $\epsilon \to +0$. Here we use such sets again, but for technical reasons we need them already in the definition of the flux. So, let $\Lambda_n \subset (-n, n)$, $n \in \mathbb{N}$, be given. We are going to make further assumption on the properties of Λ_n concerning uniform convergence below (cf. (5.6) and (5.7)). We introduce the orthogonal projections

$$P_0(\Lambda_n) = \mathcal{M}(E_{h_0}(\Lambda_n))E_{H_0}(\Lambda_n), \qquad P_1(\Lambda_n) = \mathcal{M}(E_{h_1}(\Lambda_n))E_{H_1}(\Lambda_n).$$

Since $\mathcal{M}(E_{h_0}(\Lambda_n))$ commutes with H_0 and $\mathcal{M}(E_{h_1}(\Lambda_n))$ commutes with H_1, we have $[P_j(\Lambda_n), H_j] = 0$, $j \in \{0, 1\}$. Furthermore, the relation $W_{1,\pm} = \mathcal{M}(w_{1,\pm})$ gives us $P_1(\Lambda_n)W_{1,\pm} = W_{1,\pm}P_0(\Lambda_n)$. We use $P_1(\Lambda_n)P_0(\Lambda_n)$ as identification operator to define

the wave operators

$$\begin{aligned} W_{1,\pm}(n) &= |\mathrm{A}|\text{-}\lim_{t\to\pm\infty} e^{itK_1} P_1(\Lambda_n) P_0(\Lambda_n) e^{-itK_0} P_0^{ac} \\ &= |\mathrm{A}|\text{-}\lim_{t\to\pm\infty} P_1(\Lambda_n) e^{itK_1} e^{-itK_0} P_0^{ac} P_0(\Lambda_n) = W_{1,\pm} P_0(\Lambda_n) \end{aligned}$$

for $n \in \mathbb{N}$. Similarly, let

$$P_2(\Lambda_n) = E_{H_2}(\Lambda_n).$$

Then $[P_2(\Lambda_n), H_2] = 0$ and $P_2(\Lambda_n) W_{2,\pm} P_1(\Lambda_n) = W_{2,\pm} P_1(\Lambda_n)$. We define

$$W_{2,\pm}(n) = \text{s-}\lim_{t\to\pm\infty} e^{itK_2} P_2(\Lambda_n) P_1(\Lambda_n) e^{-itK_1} = W_{2,\pm} P_1(\Lambda_n).$$

Finally, we need the stationary representations of $W_{1,\pm}(n)$ and $W_{2,\pm}(n)$. To this end, we introduce the spectral measure $E_0^{ac}(\cdot) = P_0^{ac} E_{K_0}(\cdot)$. Note that $E_{H_j}(\Xi) = E_{\varphi(H_j)}(\varphi(\Xi))$ for any $\Xi \in \mathcal{B}(\mathbb{R})$, $j \in \{0,1,2\}$, whence the definition

$$\Lambda_n^{\varphi} = \varphi(\Lambda_n) = \{\lambda \in \mathbb{R} \,|\, \lambda = \varphi(\nu), \nu \in \Lambda_n\}$$

gives us

$$P_0(\Lambda_n) = \mathcal{M}\big(E_{k_0}(\Lambda_n^{\varphi})\big) E_{K_0}(\Lambda_n^{\varphi}), \qquad P_1(\Lambda_n) = E_{K_1}(\Lambda_n^{\varphi}) \mathcal{M}\big(E_{k_1}(\Lambda_n^{\varphi})\big).$$

For $\epsilon > 0$, we set

$$\begin{aligned} W_{1,\pm}(\epsilon, n) &= \pm \int_{\mathbb{R}} i\epsilon (K_1 - \lambda \pm i\epsilon)^{-1} P_1(\Lambda_n) P_0(\Lambda_n) \mathrm{d}E_0^{ac}(\lambda) \\ &= \int_{\Lambda_n^{\varphi}} \big(1 - (K_{1,n} - \lambda \pm i\epsilon)^{-1} V_1\big) P_0(\Lambda_n) \mathrm{d}E_0^{ac}(\lambda) \end{aligned} \tag{5.4}$$

and similarly

$$W_{2,\pm}(\epsilon, n) = \int_{\Lambda_n^{\varphi}} \big(1 - (K_{2,n} - \lambda \pm i\epsilon)^{-1} V_2\big) P_1(\Lambda_n) \mathrm{d}E_{K_1}(\lambda), \tag{5.5}$$

where

$$K_{j,n} = K_j P_j(\Lambda_n), \qquad j \in \{0,1,2\}.$$

It holds that

$$W_{1,\pm}(n) = \text{s-}\lim_{\epsilon\to+0} W_{1,\pm}(\epsilon, n)$$

and

$$W_{2,\pm}(n) = \text{s-}\lim_{\epsilon\to+0} W_{2,\pm}(\epsilon, n).$$

Let $P_{0,n}^{ac} = P_0(\Lambda_n) P_0^{ac}$. We introduce the notation $\widetilde{W}_{1,\pm}(n) = P_{0,n}^{ac} - W_{1,\pm}(n)$ and

$$\widetilde{W}_{1,\pm}(\epsilon, n) = P_{0,n}^{ac} - W_{1,\pm}(\epsilon, n) = \int_{\Lambda_n^{\varphi}} (K_{1,n} - \lambda \pm i\epsilon)^{-1} V_1 P_0(\Lambda_n) \mathrm{d}E_0^{ac}(\lambda).$$

Similarly, define $\widetilde{W}_{2,\pm}(n) = P_1(\Lambda_n) - W_{2,\pm}(n)$ and

$$\widetilde{W}_{2,\pm}(\epsilon, n) = P_1(\Lambda_n) - W_{2,\pm}(\epsilon, n) = \int_{\Lambda_n^\varphi} (K_{2,n} - \lambda \pm i\epsilon)^{-1} V_2 P_1(\Lambda_n) \mathrm{d}E_{K_1}(\lambda).$$

We already used a very similar notation in Chapter 3. Note that since $V_2 \in \mathfrak{L}_1(\mathfrak{H})$, we also have $\widetilde{W}_{2,\pm}(\epsilon, n) \in \mathfrak{L}_1(\mathfrak{H})$ (cf. Lemma A.2.17).

We still have to specify the sets Λ_n, $n \in \mathbb{N}$. Similarly to the proof of Theorem 3.1.2, we use them to obtain convergence in the proof of the Landauer-Büttiker formula. The choice of the sets is also similar. Namely, choose $\Lambda_n \subset (-n, n)$ with $|(-n, n) \setminus \Lambda_n| < n^{-1}$ such that C_1 is $K_{1,n}$-smooth and

$$C_1^*(0)(K_{1,n}(0) - \lambda \pm i\epsilon)^{-1} C_1(0), \quad \int_{\mathbb{R}} \mathrm{d}\nu \, (\lambda - \nu \pm i\epsilon)^{-1} \sqrt{Y_1(\nu, 0)} \check{Q}(\nu, 0) \sqrt{Y_1(\nu, 0)}, \tag{5.6}$$

and

$$C_2(K_{2,n} - \lambda \pm i\epsilon) C_2, \quad \int_{\mathbb{R}} \mathrm{d}\nu \, (\lambda - \nu \pm i\epsilon)^{-1} \sqrt{Y_2(\nu)} \check{Q}(\nu) \sqrt{Y_2(\nu)}, \tag{5.7}$$

as well as $C_2(K_{1,n} - \lambda \pm i\epsilon)^{-1} C_1$ converge uniformly in the Hilbert-Schmidt norm for $\lambda \in \Lambda_n^\varphi$ as $\epsilon \to +0$. We introduce the definition of smoothness in Section 5.2.1 below, where we also prove that $C_2(K_{el,n} - \lambda \pm i\epsilon)^{-1} C_1$ indeed converges in the Hilbert-Schmidt norm and we find suitable sets Λ_n such that C_1 is $K_{1,n}$-smooth, c.f. Propositions 5.2.2 and 5.2.3. We already know that (5.6) and (5.7) converge by Lemmas A.2.20 and A.2.21. Hence, the existence of the sets Λ_n is guaranteed by Egorov's theorem, Lemma A.2.22. Using these sets Λ_n and the corresponding stationary wave operators, we obtain the following definition of the flux $\mathfrak{J}_Q$ of the observable Q.

Definition 5.1.7. *Let H_j, $j \in \{0, 1, 2\}$, be given by* (A0)–(A2). *For $n \in \mathbb{N}$ let Λ_n be as above. Let $Q = \mathcal{M}(q(\mu)) \in \mathfrak{B}(\mathfrak{H})$ be given by* (A4) *and define $Q_n = P_0(\Lambda_n) Q$. Let $\rho = \mathcal{M}(\rho_0 \, \delta(\mu)) \in \mathfrak{B}(\mathfrak{H})$ be given by* (A3). *Then the* flux $\mathfrak{J}_Q$ *of Q is defined by*

$$\mathfrak{J}_Q = \lim_{n \to \infty} \lim_{\epsilon \to +0} -2 \, \Im\mathrm{m}\big[\mathrm{Tr}\big(\varrho_0 W_{1,-}^*(n) W_{2,-}^*(\epsilon, n)(V_1 + V_2) Q_n W_{2,-}(\epsilon, n) W_{1,-}(n)\big)\big], \tag{5.8}$$

where $\varrho_0 = (H_0 + 1)^2 \rho$ is bounded by Assumption (A3).

Recall that we have

$$V_1 = \mathcal{M}\big((h_0 + \mu + 1)^{-1} - (h_1 + \mu + 1)^{-1}\big),$$

where the resolvent difference satisfies $(h_0 + \mu + 1)^{-1} - (h_1 + \mu + 1)^{-1} \in \mathfrak{L}_1(\mathfrak{h})$ for $\mu \geq 0$ and $W_{1,\pm}(n) = W_{1,\pm} P_0(\Lambda_n)$ with $W_{1,-}^* = \mathcal{M}(w_{1,-}^*)$. Also, $\rho(\mu) = \rho_0 \, \delta(\mu)$. Since ϱ_0 commutes with $E_{K_0}(\cdot)$ and $\mathcal{M}\big(E_{k_0}(\cdot)\big)$, this implies that

$$\varrho_0 W_{1,\pm}^*(n) V_1 = P_0(\Lambda_n)(H_0 + 1)^2 \mathcal{M}\big(\rho_0 w_{1,\pm} v_1 \delta(\mu)\big) \in \mathfrak{L}_1(\mathfrak{H}).$$

Furthermore, $V_2 \in \mathfrak{L}_1(\mathfrak{H})$ and $\widetilde{W}_{2,-} \in \mathfrak{L}_1(\mathfrak{H})$, whence the flux is indeed well-defined.

We can derive this definition from the formal expression for the current using the cyclicity of the trace, $[K_0, Q] = 0$, the intertwining property of the wave operators, and

$W_-(H_2, H_0) = W_{2,-}W_{1,-}$. Note that $W_{j,\pm} = \text{s-lim}_{n\to\infty} W_{j,\pm}(n)$, $j \in \{1,2\}$. We get, formally,

$$\begin{aligned} &i\,\mathrm{Tr}\big(W_-(H_2,H_0)\rho\, W_-^*(H_2,H_0)[H_2,Q]\big) \\ &= \lim_{n\to\infty} i\,\mathrm{Tr}\big(\varrho_0 W_{1,-}^*(n)W_{2,-}^*(n)(H_2+1)^{-1}[H_2,Q_n](H_2+1)^{-1}W_{2,-}(n)W_{1,-}(n)\big). \end{aligned}$$

Thus,

$$\begin{aligned} &i\,\mathrm{Tr}\big(W_-(H_2,H_0)\rho\, W_-^*(H_2,H_0)[H_2,Q]\big) \\ &= \lim_{n\to\infty}\lim_{\epsilon\to+0} -i\,\mathrm{Tr}\big(\varrho_0 W_{1,-}^*(n)W_{2,-}^*(\epsilon,n)[(H_2+1)^{-1},Q_n]W_{2,-}(\epsilon,n)W_{1,-}(n)\big) \\ &= \lim_{n\to\infty}\lim_{\epsilon\to+0} i\,\mathrm{Tr}\big(\varrho_0 W_{1,-}^*(n)W_{2,-}^*(\epsilon,n)(V_1+V_2)Q_nW_{2,-}(\epsilon,n)W_{1,-}(n)\big) \\ &\qquad\qquad - i\,\mathrm{Tr}\big(\varrho_0 W_{1,-}^*(n)W_{2,-}^*(\epsilon,n)Q_n(V_1+V_2)W_{2,-}(\epsilon,n)W_{1,-}(n)\big) \\ &= \lim_{n\to\infty}\lim_{\epsilon\to+0} -2\,\Im\mathrm{m}\big[\mathrm{Tr}\big(\varrho_0 W_{1,-}^*(n)W_{2,-}^*(\epsilon,n)(V_1+V_2)Q_nW_{2,-}(\epsilon,n)W_{1,-}(n)\big)\big]. \end{aligned}$$

The order of the limits $n \to \infty$ and $\epsilon \to +0$ is the reason why we have to use the sets Λ_n already in the definition of the flux. The regularization $\epsilon \to +0$ is necessary to obtain well-defined traces. The regularization $n \to \infty$ is necessary to obtain uniform convergence as $\epsilon \to +0$ in the proof, whence we can not easily interchange it with the limit $n \to \infty$.

Recall that the definition of the flux derives from the relation $\omega(\mathrm{d}\Gamma(A)) = \mathrm{Tr}(\rho A)$, cf. (A.1.9). However, this formula holds only if A is trace class. In the abstract Landauer-Büttiker formula of Chapter 3, the flux observable

$$A = (H+\theta)^{-N_Q}[(H_0+\theta)^{-N} - (H+\theta)^{-N}, Q](H+\theta)^{-N_Q} \in \mathfrak{L}_1(\mathfrak{H})$$

does indeed satisfy this requirement. In this chapter, however, the flux observable is not trace class. The trace class condition is only satisfied together with the initial state ρ. Thus, the definition of the flux is not strictly derived from the principles of second quantization as in the case of Definition 3.1.1. Nevertheless, it is still strongly related to the concept of second quantization and thus far more than a heuristic definition since

$$\lim_{m\to\infty} \omega(\mathrm{d}\Gamma(A_m)) = \mathrm{Tr}(\rho A)$$

holds if $A = \text{s-lim}_{m\to\infty} A_m$ for $A_m \in \mathfrak{L}_1(\mathfrak{H})$ and $\rho A_m \to \rho A$ in the trace norm.

With this definition of the flux, we can prove the Landauer-Büttiker formula we have already mentioned. Let again $S(\lambda)$ and $T(\lambda)$ denote the scattering matrix respectively the transition matrix of the scattering system $\{H_0, H_2\}$ with respect to a spectral representation Φ_{H_0} of H_0^{ac}.

Theorem 5.1.8. *Let H_j, $j \in \{0,1,2\}$, be given by* (A0)–(A2). *For $n \in \mathbb{N}$ let Λ_n be as above. Let $Q = \mathcal{M}(q(\mu)) \in \mathfrak{B}(\mathfrak{H})$ be given by* (A4) *and define $Q_n = P_0(\Lambda_n)Q$. Let $\rho = \mathcal{M}(\rho_0\,\delta(\mu)) \in \mathfrak{B}(\mathfrak{H})$ be given by* (A3). *Then*

$$\mathfrak{J}_Q = \frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{d}\lambda \mathrm{Tr}\Big(\rho(\lambda)(S^*(\lambda)Q(\lambda)S(\lambda) - Q(\lambda))\Big).$$

5.2 Proof of Theorem 5.1.8

The idea of the proof is the following. In the first part, Section 5.2.1, we introduce the notion of H-smoothness of an operator for a Hamiltonian H. We use this to show the existence of the limits $C_1(K_{1,n} - \lambda \pm i0)^{-1}C_2$ in the Hilbert-Schmidt norm. We need this in the final part of the proof. The main idea of the proof is the same as in the proof of the Landauer-Büttiker formula of Chapter 3. The main difference is that we can not work with the transition matrix $T(\lambda)$ for the scattering system $\{H_0, H_2\}$, because we do not have $(H_2+1)^{-1} - (H_0+1)^{-1} \in \mathfrak{L}_1(\mathfrak{H})$. Hence, in Section 5.2.2 we construct spectral representations of K_0^{ac} and K_1, and we obtain formulae for the transition matrices $\check{T}_1(\lambda)$ and $\check{T}_2(\lambda)$ of the scattering systems $\{K_0, K_1\}$ and $\{K_1, K_2\}$, respectively. Since H_0 and H_1 are multiplication operators, we work in the fiber for $\check{T}_1(\lambda)$.

The actual proof follows in Section 5.2.3. First we reduce the problem from the Hamiltonians H_j to the resolvents K_j, $j \in \{0, 1, 2\}$. The two scattering systems $\{K_0, K_1\}$ and $\{K_1, K_2\}$ lead to a decomposition of the flux $\mathfrak{J}_Q$ into four parts, Σ_1–Σ_4. We calculate the contributions of these parts in four separate lemmas. The calculations of Σ_3 and Σ_4 are more complicated than the rest and require some technical lemmas that we also proof in Section 5.2.3. The Landauer-Büttiker formula is then simply the result of adding up the contributions of Σ_1–Σ_4.

5.2.1 Smoothness

In Section 3.1 the proof of the usual Landauer-Büttiker formula for relatively trace class perturbations uses the existence of the limits $\lim_{\epsilon\to+0} C^*(H-\lambda\pm i\epsilon)^{-1}C$, which we obtain form the fact that C is a Hilbert-Schmidt operator. For the Landauer-Büttiker formula for multiplication operators, we need similar limits, but only $C_1(\mu)$, $\mu \geq 0$, is Hilbert-Schmidt and this does not survive the transition from the fiber to the whole space, i.e. C_1 is not Hilbert-Schmidt. A notion that gives us the existence of the necessary limits is that of smoothness (cf. [80]). Since it is sufficient in our case, we state the definition of smoothness only for bounded operators.

Definition 5.2.1. *Let H be a self-adjoint operator on $\mathrm{dom}(H) \subset \mathfrak{H}$. An operator $X_1 \in \mathfrak{B}(\mathfrak{H})$ is called* H-smooth*, if*

$$\sup_{\Xi\in\mathcal{B}(\mathbb{R})} |\Xi|^{-1}\|X_1 E_H(\Xi)\|^2 < \infty.$$

We are interested in the existence of the limits $\lim_{\epsilon\to+0} C_1(K_{1,n} - \lambda \pm i\epsilon)^{-1}C_2$ (used in Lemma 5.2.12). First we show that these limits exist if C_1 is $K_{1,n}$-smooth and C_2 is Hilbert-Schmidt. Since we already know that C_2 is indeed Hilbert-Schmidt, it suffices to verify the smoothness condition for C_1, which is done in Proposition 5.2.3.

Proposition 5.2.2. *Let H be a densely defined self-adjoint operator on $\mathfrak{H}$. Let further $X_1 \in \mathfrak{B}(\mathfrak{H})$ be H-smooth and $X_2 \in \mathfrak{L}_2(\mathfrak{H})$. Then for a.e. $\lambda \in \mathbb{R}$ the limits*

$$\lim_{\epsilon\to+0} X_1(H - \lambda \pm i\epsilon)^{-1}X_2$$

exist in $\mathfrak{L}_2(\mathfrak{H})$.

Proof. Choose an open bounded set $\Xi \in \mathcal{B}(\mathbb{R})$. Then for every $\lambda \in \Xi$,

$$(H - \lambda \pm i\epsilon)^{-1} = (HE_H(\Xi) - \lambda \pm i\epsilon)^{-1} + (HE_H(\mathbb{R} \setminus \Xi) - \lambda \pm i\epsilon)^{-1} - (\lambda \pm i\epsilon)^{-1}$$

and the limit of the second summand exists since $\Xi \cap \sigma\big(HE_H(\mathbb{R} \setminus \Xi)\big) = \emptyset$. The limit of $(\lambda \pm i\epsilon)^{-1}$ exists trivially for $\lambda \neq 0$. Hence, it is sufficient to prove the proposition for bounded H. Let now H be bounded. Note that $X_1 E_H(\Xi) X_2 \in \mathfrak{L}_2(\mathfrak{H})$ for $\Xi \in \mathcal{B}(\mathbb{R})$. Furthermore, E_H is zero outside the bounded set $\sigma(H)$. Let $\mathcal{J}(H)$ denote any partition of $\sigma(H)$. It follows that the total variation of $X_1 E_H(\cdot) X_2$ as a vector measure with values in $\mathfrak{L}_2(\mathfrak{H})$ is

$$\begin{aligned}
&\sup_{\mathcal{J}(H)} \sum_{\Xi \in \mathcal{J}(H)} \|X_1 E_H(\Xi) X_2\|_2 \\
&\quad \leq \sup_{\mathcal{J}(H)} \sum_{\Xi \in \mathcal{J}(H)} |\Xi|^{\frac{1}{2}} |\Xi|^{-\frac{1}{2}} \|X_1 E_H(\Xi)\| \, \|E_H(\Xi) X_2\|_2 \\
&\quad \leq \sup_{\mathcal{J}(H)} \Big(\sum_{\Xi \in \mathcal{J}(H)} |\Xi| |\Xi|^{-1} \|X_1 E_H(\Xi)\|^2 \Big)^{\frac{1}{2}} \Big(\sum_{\Xi \in \mathcal{J}(H)} \|E_H(\Xi) X_2\|_2^2 \Big)^{\frac{1}{2}}.
\end{aligned}$$

By Definition 5.2.1, we have $\sup_{\Xi \in \mathcal{B}(\mathbb{R})} |\Xi|^{-1} \|X_1 E_H(\Xi)\|^2 < \infty$, whence

$$\sup_{\mathcal{J}(H)} \sum_{\Xi \in \mathcal{J}(H)} \|X_1 E_H(\Xi) X_2\|_2 \leq \sup_{\mathcal{J}(H)} \Big(\sum_{\Xi \in \mathcal{J}(H)} |\Xi| \Big)^{\frac{1}{2}} \widetilde{\gamma} \, \|X_2\|_2 = \widetilde{\gamma} \, |\sigma(H)|^{\frac{1}{2}} \|X_2\|_2$$

for some $\widetilde{\gamma} > 0$. Since we assumed that H is bounded, $X_1 E_H(\cdot) X_2$ is a vector measure with finite total variation that takes values in the Hilbert space $\mathfrak{L}_2(\mathfrak{H})$. Thus, it follows from [9, Prop. I.1.2] that

$$\lim_{\epsilon \to +0} X_1 \big(H - \lambda \pm i\epsilon\big)^{-1} X_2 = \lim_{\epsilon \to +0} \int_{\mathbb{R}} \frac{1}{\nu - \lambda \pm i\epsilon} \, \mathrm{d} X_1 E_H(\varphi(\nu)) X_2$$

exists in the Hilbert-Schmidt norm for a.e. $\lambda \in \mathbb{R}$. □

Proposition 5.2.3. *For every $n \in \mathbb{N}$ and $\epsilon > 0$, one can find a set $\Lambda_n \subset (-n, n)$ satisfying $|(-n, n) \setminus \Lambda_n| < \epsilon n^{-1}$ such that C_1 is $K_{1,n}$-smooth.*

Proof. First we prove that C_1 is $H_{1,n}$-smooth. Note that since c_1 is a Hilbert-Schmidt operator, for any $\epsilon > 0$ there is a set $\Lambda_n \subset (-n, n)$ satisfying $|(-n, n) \setminus \Lambda_n| < \epsilon n^{-1}$ such that c_1 is $h_{1,n}$-smooth, where $h_{1,n} = h_1 E_{h_1}(\Lambda_n)$. This follows from the fact that Hilbert-Schmidt operators are integral operators, and integral operators with an essentially bounded kernel are smooth by [9, Thm. IV.17.12]. Furthermore, $[D_1(\mu), h_1] = 0$ and $\|D_1(\mu)\| \leq 1$ for $\mathfrak{m}$-a.e. $\mu \geq 0$. Hence,

$$\begin{aligned}
\sup_{\Xi \subset \mathbb{R}} |\Xi|^{-1} \|C_1 E_{H_{1,n}}(\Xi)\|^2 &= \sup_{\Xi \subset \mathbb{R}} \sup_{\mu \geq 0} |\Xi|^{-1} \|c_1 D_1(\mu) E_{H_{1,n}(\mu)}(\Xi)\|^2 \\
&\leq \sup_{\mu \geq 0} \sup_{\Xi \subset \mathbb{R}} |\Xi|^{-1} \|c_1 E_{h_{1,n}}(\Xi - \mu)\|^2.
\end{aligned}$$

Since the Lebesgue measure is translation invariant, this gives us

$$\sup_{\Xi\subset\mathbb{R}}|\Xi|^{-1}\|C_1E_{H_{1,n}}(\Xi)\|^2=\sup_{\mu\geq 0}\sup_{\Xi\subset\mathbb{R}}|\Xi-\mu|^{-1}\|c_1E_{h_{1,n}}(\Xi)\|^2<\infty.$$

Thus, C_1 is $H_{1,n}$-smooth. Note that in the above estimate it is important that c_1, the 'Hilbert-Schmidt part' of $C_1(\mu)$, is independent of μ. This uniformity allows us to drop the supremum over μ.

Now we show that C_1 is also $K_{1,n}$-smooth. For $\Xi\in\mathcal{B}(\mathbb{R})\cap\sigma(K_{1,n})$, we have

$$E_{K_{1,n}}(\Xi)=E_{H_{1,n}}(\varphi^{-1}(\Xi)),$$

where $\varphi^{-1}(\nu)=-\nu^{-1}-1$ for $\nu\in\sigma(K_{1,n})$. It follows that

$$\begin{aligned}&\sup_{\Xi\in\mathcal{B}(\mathbb{R})\cap\sigma(K_{1,n})}|\Xi|^{-1}\|C_1E_{K_{1,n}}(\Xi)\|\\&\quad=\sup_{\Xi\in\mathcal{B}(\mathbb{R})\cap\sigma(K_{1,n})}|\Xi|^{-1}|\varphi^{-1}(\Xi)||\varphi^{-1}(\Xi)|^{-1}\|C_1E_{H_{1,n}}(\varphi^{-1}(\Xi))\|\\&\quad=\sup_{\Xi\in\mathcal{B}(\mathbb{R})\cap\sigma(H_{1,n})}|\Xi||\varphi(\Xi)|^{-1}|\Xi|^{-1}\|C_1E_{H_{el,n}}(\Xi)\|\end{aligned}$$

for $\varphi(\nu)=-(\nu+1)^{-1}$. Since $\sigma(H_{1,n})\subset(-n,n)$ is a bounded set, $\frac{\mathrm{d}}{\mathrm{d}\nu}\varphi(\nu)=\varphi(\nu)^2\geq\gamma$ for every $\nu\in\sigma(H_{1,n})$ and some $\gamma>0$, we obtain

$$\sup_{\Xi\in\mathcal{B}(\mathbb{R})\cap\sigma(K_{1,n})}|\Xi||\varphi(\Xi)|^{-1}\leq\widetilde{\gamma}$$

for some $\widetilde{\gamma}>0$. Thus, using that C_1 is $H_{1,n}$-smooth, we conclude the proof with the estimate

$$\sup_{\Xi\in\mathcal{B}(\mathbb{R})\cap\sigma(K_{1,n})}|\Xi|^{-1}\|C_1E_{K_{1,n}}(\Xi)\|\ \leq\sup_{\Xi\in\mathcal{B}(\mathbb{R})\cap\sigma(H_{1,n})}\widetilde{\gamma}\,|\Xi|^{-1}\|C_1E_{H_{1,n}}(\Xi)\|<\infty.$$

□

5.2.2 Spectral representation and transition matrix

The proof of Theorem 5.1.8 follows the same lines as the one for the Landauer-Büttiker formula for trace class perturbations, Theorem 3.1.2. This is why this section is dedicated to spectral representations of K_0^{ac} and K_1 and formulae for the transition matrices $\breve{T}_1(\lambda)$ and $\breve{T}_2(\lambda)$, $\lambda\in\mathbb{R}$.

The flux of Q is defined using $K_j=-(H_j+1)^{-1}$, $j\in\{0,1,2\}$, whence we can use the fact that the resolvent differences $K_1(\mu)-K_0(\mu)=(H_0(\mu)+1)^{-1}-(H_1(\mu)+1)^{-1}$ for $\mathfrak{m}$-a.e. $\mu\geq 0$, and $V_2=(H_1+1)^{-1}-(H_2+1)^{-1}$ are trace class. Recall that trace class perturbations give rise to special spectral representation by Lemma 3.1.4. The resolvent difference $V_1=\mathcal{M}(V_1(\mu))=(H_0+1)^{-1}-(H_1+1)^{-1}$ itself is not trace class, but it is a multiplication operator with a trace class-valued function. For $\mathfrak{m}$-a.e. $\mu\geq 0$ let $E^{ac}_{K_0(\mu)}$

be the spectral measure of $K_0^{ac}(\mu)$, the absolutely continuous part of $K_0(\mu)$, and let

$$Y_1(\lambda,\mu) = \frac{\mathrm{d}}{\mathrm{d}\lambda} C_1(\mu) E_{K_0(\mu)}(\lambda) C_1^*(\mu).$$

For $\mathfrak{m}$-a.e. fiber $\mu \geq 0$, we obtain a spectral representation $\Phi_{K_0}(\mu)$ of $K_0^{ac}(\mu)$ on the direct integral $L^2(\mathbb{R}, \mathrm{d}\lambda, \mathfrak{h}_\lambda(\mu))$ from Lemma 3.1.4. We want to raise this spectral representation in the fiber to a spectral representation of $K_{0,ac} = K_0 P_0^{ac}$. The following Lemma gives us the spectral measures of K_0 and K_1.

Lemma 5.2.4. *Let $j \in \{0,1\}$, and let $E_{K_j(\mu)}$ be the spectral measure of $K_j(\mu)$. Then the spectral measure of $K_j = \mathcal{M}(K_j(\mu))$ is given by*

$$E_{K_j}(\Xi) = \mathcal{M}(E_{K_j(\mu)}(\Xi))$$

for $\Xi \in \mathcal{B}(\mathbb{R})$.

Proof. Let $j \in \{0,1\}$. It is obvious that $\mathcal{M}(E_{K_j(\mu)}(\cdot))$ is a spectral measure. Furthermore,

$$\Big(\sum_{n=0}^{N} \lambda_n \mathcal{M}(E_{K_j(\mu)}(\Xi_n)) f\Big)(\mu) = \sum_{n=0}^{N} \lambda_n E_{K_j(\mu)}(\Xi_n) f(\mu),$$

whence

$$\Big(\int_{\mathbb{R}} \lambda \,\mathrm{d}\mathcal{M}(E_{K_j(\mu)}(\lambda)) f\Big)(\mu) = \int_{\mathbb{R}} \lambda \,\mathrm{d}E_{K_j(\mu)}(\lambda) f(\mu) = K_j(\mu) f(\mu) = (K_j f)(\mu)$$

for all $f \in \mathfrak{H}$ and $\mathfrak{m}$-a.e. $\mu \geq 0$. □

Note that

$$E_{k_0}(\Lambda_n^\varphi) = E_{h_0}(\Lambda_n) = E_{H_0(\mu)}(\Lambda_n + \mu) = E_{K_0(\mu)}(\varphi(\Lambda_n + \mu))$$

for any $\mu \geq 0$. It follows that

$$P_0(\Lambda_n) = \mathcal{M}\big((E_{k_0}(\Lambda_n^\varphi)) E_{K_0}(\Lambda_n^\varphi) = \mathcal{M}\big(E_{K_0(\mu)}(\Lambda_n^\varphi(\mu))\big),$$

where

$$\Lambda_n^\varphi(\mu) = \Lambda_n^\varphi \cap \varphi(\Lambda_n + \mu)$$

for $\mu \geq 0$. Hence,

$$K_{0,n} = \mathcal{M}\big(K_0(\mu) E_{K_0(\mu)}(\Lambda_n^\varphi(\mu))\big), \qquad K_{1,n} = \mathcal{M}\big(K_1(\mu) E_{K_1(\mu)}(\Lambda_n^\varphi(\mu))\big).$$

It follows that the stationary pre-wave operators $W_{1,\pm}(\epsilon, n)$ are also multiplication operators and

$$W_{1,\pm}(\epsilon, n) = \mathcal{M}\Big(\int_{\Lambda_n^\varphi} (1 - (K_{1,n}(\mu) - \lambda \pm i\epsilon)^{-1} V_1(\mu)) E_{K_0(\mu)}(\Lambda_n^\varphi(\mu)) \mathrm{d}E_{K_0(\mu)}^{ac}(\lambda)\Big).$$

Since $E_{K_0}^{ac} \neq \mathcal{M}(E_{K_0(\mu)}^{ac})$, we work with the measure

$$E_0^{ac} = P_0^{ac} E_{K_0}^{ac} = \mathcal{M}(E_{K_0(\mu)}^{ac})$$

and the Hilbert space $\mathfrak{H}_0^{ac} = P_0^{ac}\mathfrak{H}$. As an easy consequence of Lemma 5.2.4, we obtain a spectral representation of $K_{0,ac}$ from $\Phi_{K_0}(\mu)$, $\mu \geq 0$. Let $L^2(\mathbb{R}, \mathrm{d}\lambda, \mathfrak{h}_\lambda(\mu))$ be the direct integral of the spectral representation $\Phi_{K_0}(\mu)$.

Lemma 5.2.5. *A spectral representation Φ_{K_0} of $K_{0,ac}$ on*

$$\mathfrak{H}_{\Phi_{K_0}} = L^2(\mathbb{R}, \mathrm{d}\lambda, \mathfrak{H}_\lambda), \qquad \mathfrak{H}_\lambda = L^2(\mathbb{R}_+^0, \mathrm{d}\mathfrak{m}(\mu), \mathfrak{h}_\lambda(\mu))$$

is given by

$$\big((\Phi_{K_0} f)(\lambda)\big)(\mu) = \big(\Phi_{K_0}(\mu) f(\mu)\big)(\lambda)$$

for $f \in \mathfrak{H}_0^{ac}$.

Proof. We have

$$\|\Phi_{K_0} f\|^2 = \int_{\mathbb{R}} \mathrm{d}\mathfrak{m}(\mu) \int_{\mathbb{R}} \mathrm{d}\lambda \, \|(\Phi_{K_0}(\mu) f(\mu))(\lambda)\|^2 = \int_{\mathbb{R}} \mathrm{d}\mathfrak{m}(\mu) \|f(\mu)\|^2 = \|f\|^2,$$

whence Φ_{K_0} is an isometry. Let $\check{g} \in \mathfrak{H}_{\Phi_{K_0}}$. We define $g \in \mathfrak{H}_0^{ac}$ by

$$g(\mu) = \Phi_{K_0}^*(\mu) \check{g}(\cdot, \mu)$$

for $\mathfrak{m}$-a.e. $\mu \geq 0$. Then

$$(\Phi_{K_0} g)(\lambda, \mu) = \big(\Phi_{K_0}(\mu) \Phi_{K_0}^*(\mu) \check{g}(\cdot, \mu)\big)(\lambda) = \check{g}(\lambda, \mu)$$

for a.e. $\lambda \in \mathbb{R}$ and $\mathfrak{m}$-a.e. $\mu \geq 0$. Thus, Φ_{K_0} is also surjective and hence unitary. Furthermore,

$$\begin{aligned} \Big(\big(\mathcal{M}(\Phi_{K_0}(\mu)) K_0 f\big)(\mu)\Big)(\lambda) &= \big(\Phi_{K_0}(\mu) K_0(\mu) f(\mu)\big)(\lambda) \\ &= \lambda\big(\Phi_{K_0}(\mu) f(\mu)\big)(\lambda) \\ &= \lambda\Big(\big(\mathcal{M}(\Phi_{K_0}(\mu)) f\big)(\mu)\Big)(\lambda), \end{aligned}$$

whence Φ_{K_0} is indeed a spectral representation and the lemma is proven. □

Recall from the proof of the Landauer-Büttiker formula, Theorem 3.1.2, that operators of the form

$$L = \int_{\mathbb{R}} \mathrm{d}E_0^{ac}(\nu) C_1^* X(\nu) \tag{5.9}$$

with a family of functions $\{X(\nu)\}_{\nu \in \mathbb{R}}$ play an important part. They originate from the stationary representation of the wave operators. The following lemma tells us that if $X(\nu)$ is a multiplication operator, then these operators are in turn multiplication operators and simply act on each fiber of $\mathfrak{H} = L^2(\mathbb{R}_+^0, \mathrm{d}\mathfrak{m}(\mu), \mathfrak{h})$.

Lemma 5.2.6. *Let $X(\nu) : \mathbb{R} \to \mathfrak{B}(\mathfrak{H})$ be given, where $X(\nu) = \mathcal{M}(X(\nu,\mu))$ with $X(\nu,\mu) \in \mathfrak{B}(\mathfrak{h})$, and assume that the operator spectral integral given by (5.9) exists and is denoted by L. Then for $\mathfrak{m}$-a.e. $\mu \geq 0$ and all $f \in \mathfrak{H}$,*

$$(Lf)(\mu) = L(\mu)f(\mu) = \int_{\mathbb{R}} \mathrm{d}E^{ac}_{K_0(\mu)}(\nu) C_1^* X(\nu,\mu) f(\mu).$$

Proof. From the definition of the operator spectral integral, we obtain

$$g = \int_{-r}^{r} \mathrm{d}E^{ac}_0(\nu) C_1^* X(\nu) f = \operatorname*{s-lim}_{\epsilon \to +0} \sum_{\Xi_\epsilon \in \mathcal{J}^r_\epsilon} E^{ac}_0(\Xi_\epsilon) C_1^* X(\nu_{\Xi_\epsilon}) f$$

for any $f \in \mathfrak{H}$, $r > 0$, $\epsilon > 0$, and any partition $\mathcal{J}^r_\epsilon$ of $(-r, r)$ with $|\mathcal{J}^r_\epsilon| = \epsilon$, where $\nu_{\Xi_\epsilon} \in \Xi_\epsilon$ for every $\Xi_\epsilon \in \mathcal{J}^r_\epsilon$. Thus, Lemma 5.2.4 implies

$$\begin{aligned}
&\lim_{\epsilon \to +0} \Big\| g - \sum_{\Xi_\epsilon \in \mathcal{J}^r_\epsilon} E^{ac}_0(\Xi_\epsilon) C_1^* X(\nu_{\Xi_\epsilon}) f \Big\|^2_{L^2\left(\mathbb{R}, \mathrm{d}\mathfrak{m}(\mu), \mathfrak{h}\right)} \\
&\quad = \int_{\mathbb{R}} \mathrm{d}\mathfrak{m}(\mu) \Big\| g(\mu) - \sum_{\Xi_\epsilon \in \mathcal{J}^r_\epsilon} E^{ac}_{K_0(\mu)}(\Xi_\epsilon) C_1^* X(\nu_{\Xi_\epsilon}, \mu) f(\mu) \Big\|^2 = 0.
\end{aligned}$$

It follows that

$$g(\mu) = \lim_{\epsilon \to +0} \sum_{\Xi_\epsilon \in \mathcal{J}^r_\epsilon} E^{ac}_{K_0(\mu)}(\Xi_\epsilon) C_1^* X(\nu_{\Xi_\epsilon}, \mu) f(\mu) = \int_{-r}^{r} \mathrm{d}E^{ac}_{K_0(\mu)}(\nu) C_1^* X(\nu,\mu) f(\mu)$$

for $\mathfrak{m}$-a.e. $\mu \geq 0$. The lemma follows if we take the limit $r \to \infty$. □

The following lemma gives us the action of Φ_{K_0} on L.

Lemma 5.2.7. *Let $X(\nu) : \mathbb{R} \to \mathfrak{B}(\mathfrak{H})$ with $X(\nu) = \mathcal{M}(X(\nu,\mu))$, $X(\nu,\mu) \in \mathfrak{B}(\mathfrak{h})$, be strongly continuous and assume that the operator spectral integral given by*

$$L = \int_{\mathbb{R}} \mathrm{d}E^{ac}_0(\nu) C_1^* X(\nu)$$

exists. Then

$$(\Phi_{K_0} L f)(\lambda) = \sqrt{Y_1(\lambda)} X(\lambda) f \tag{5.10}$$

holds, where $\sqrt{Y_1(\lambda)} = \mathcal{M}\big(\sqrt{Y_1(\lambda,\mu)}\big)$. Furthermore, for $g \in \mathfrak{H}^{ac}_0$

$$L^* g = \int_{\mathbb{R}} \mathrm{d}\lambda\, X^*(\lambda) \sqrt{Y_1(\lambda)} \check{g}(\lambda). \tag{5.11}$$

Proof. Let $f \in \mathfrak{H}$. By Lemma 5.2.6 we have

$$\begin{aligned}
(L_r f)(\mu) &= \int_{-r}^{r} \mathrm{d}E^{ac}_{K_0(\mu)} C_1^* X(\nu,\mu) f(\mu) \\
&= \lim_{\epsilon \to +0} \sum_{\Xi_\epsilon \in \mathcal{J}^r_\epsilon} E^{ac}_{K_0(\mu)}(\Xi_\epsilon) C_1^* X(\nu_{\Xi_\epsilon}, \mu) f(\mu)
\end{aligned}$$

for $r > 0$. Using Lemma 3.1.4 and Corollary 5.2.5 leads to

$$\begin{aligned}(\Phi_{K_0} L_r f)(\lambda,\mu) &= \lim_{\epsilon\to+0} \sum_{\Xi_\epsilon\in\mathcal{J}_\epsilon^r} \Big(\Phi_{K_0}(\mu) E^{ac}_{K_0(\mu)}(\Xi_\epsilon) C_1^*(\mu) X(\nu_{\Xi_\epsilon},\mu) f(\mu)\Big)(\lambda) \\ &= \lim_{\epsilon\to+0} \sum_{\Xi_\epsilon\in\mathcal{J}_\epsilon^r} \chi_{\Xi_\epsilon}(\lambda)\sqrt{Y_1(\lambda,\mu)}X(\nu_{\Xi_\epsilon},\mu) f(\mu) \\ &= \lim_{\epsilon\to+0} \sqrt{Y_1(\lambda,\mu)}X(\nu^\lambda_{\Xi_\epsilon},\mu) f(\mu) \\ &= \sqrt{Y_1(\lambda,\mu)}X(\lambda,\mu) f(\mu)\end{aligned}$$

for every $\lambda \in (-r, r)$, where $\Xi^\lambda_{\epsilon,r}$ is the unique element of $\mathcal{J}^r_\epsilon$ for which $\lambda \in \Xi^\lambda_{\epsilon,r}$. It remains to take the limit $r \to \infty$ to obtain (5.10). The adjoint relation (5.11) follows easily from

$$\begin{aligned}\langle f, L^* g\rangle = \langle Lf, g\rangle &= \langle \Phi_{K_0} Lf, \Phi_{K_0} g\rangle \\ &= \int_{\mathbb{R}} \mathrm{d}\mathfrak{m}(\mu) \int_{\mathbb{R}} \mathrm{d}\lambda \left\langle \sqrt{Y_1(\lambda,\mu)}X(\lambda,\mu) f(\mu), \check{g}(\lambda,\mu)\right\rangle \\ &= \int_{\mathbb{R}} \mathrm{d}\mathfrak{m}(\mu) \Big\langle f(\mu), \int_{\mathbb{R}} \mathrm{d}\lambda\, X^*(\lambda,\mu)\sqrt{Y_1(\lambda,\mu)}\check{g}(\lambda,\mu)\Big\rangle \\ &= \Big\langle f, \int_{\mathbb{R}} \mathrm{d}\lambda\, X^*(\lambda)\sqrt{Y_1(\lambda)}\check{g}(\lambda)\Big\rangle\end{aligned}$$

for all $f, g \in \mathfrak{H}_0^{ac}$. □

The Landauer-Büttiker formula (5.8) can be reformulated as

$$\begin{aligned}\mathfrak{J}_Q &= \frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{d}\lambda \mathrm{Tr}\Big(\rho(\lambda)(S^*(\lambda)Q(\lambda)S(\lambda) - Q(\lambda))\Big) \\ &= -2\pi \int_{\mathbb{R}} \mathrm{d}\lambda \mathrm{Tr}\Big(\rho(\lambda)(T^*(\lambda)T(\lambda)Q(\lambda) - T^*(\lambda)Q(\lambda)T(\lambda)) \\ &\qquad\qquad + (2\pi i)^{-1} T(\lambda)[Q(\lambda),\rho(\lambda)]\Big),\end{aligned}$$

where $S = W_+^*(H_2, H_0)W_-(H_2, H_0)$ and $T = P_0^{ac} - 2\pi i\, S$ is the transition operator of the scattering system $\{H_0, H_2\}$. Recall that we can use the chain rule for wave operators and the invariance principle to write $W_\pm(H_2, H_0)$ as the product of $W_{2,\pm}$ and $W_{1,\pm}$. Using the definition $S_2 = W_{2,+}^* W_{2,-} = I_{\mathfrak{H}} - 2\pi i\, T_2$, we get

$$T = \tfrac{1}{2\pi i}(P_0^{ac} - W_{1,+}^* W_{2,+}^* W_{2,-} W_{1,-}) = T_1 + W_{1,+}^* T_2 W_{1,-}.$$

Note that since T_1 commutes with H_0, it also commutes with K_0 and we get a transition matrix $\check{T}_1(\lambda)$ with respect to the spectral representation Φ_{K_0}. Similarly, T_2 commutes with H_1 and hence with K_1, and we obtain the transition matrix $\check{T}_2(\lambda)$ with respect to Φ_{K_1}, where Φ_{K_1} is the spectral representation of K_1 that we obtain from

$$Y_2(\lambda) = \frac{\mathrm{d}}{\mathrm{d}\lambda} C_2 E_{K_1}(\lambda) C_2$$

and Lemma 3.1.4. Now $\Phi_{K_1} W_{1,\pm} \Phi_{K_0}^* = \mathcal{M}(\check{W}_{1,\pm}(\lambda))$, whence

$$\check{T}(\lambda) = \check{T}_1(\lambda) + \check{W}_{1,+}^*(\lambda)\breve{T}_2(\lambda)\check{W}_{1,-}(\lambda)$$

for every $f \in \mathfrak{H}_0^{ac}$. We can prove a formula for $\breve{T}_2(\lambda)$ that is similar to Proposition 3.1.6 but includes the identification operator. Recall that $P_1(\Lambda_n) = \mathcal{M}(E_{K_1(\mu)}(\Lambda_n^\varphi(\mu)))$ with $\Lambda_n^\varphi(\mu) \subset (-n, n)$ for $n \in \mathbb{N}$.

Proposition 5.2.8. *For a.e. $\lambda \in \mathbb{R}$ the transition matrix $\breve{T}_2(\lambda)$ for $W_{2,\pm}$ with respect to Φ_{K_1} satisfies*

$$\breve{T}_2(\lambda)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda)) = \sqrt{Y_2(\lambda)}J_{2,n}(\lambda + i0)\sqrt{Y_2(\lambda)}\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda)), \tag{5.12}$$

where

$$J_{2,n}(\lambda + i0) = \lim_{\epsilon \to +0} Z_2 - Z_2 C_2 (K_{2,n} - \lambda - i\epsilon)^{-1} C_2 Z_2$$

and the limit is taken in the Hilbert-Schmidt norm.

Proof. The proof is very similar to the proof of Proposition 3.1.6. Recall that we have $W_{2,\pm}(n) = W_{2,\pm} P_1(\Lambda_n)$ and

$$\big(\Phi_1 P_1(\Lambda_n) g\big)(\lambda, \mu) = \big(\Phi_1 \mathcal{M}(E_{K_1(\mu)}(\Lambda_n^\varphi(\mu)))g\big)(\lambda, \mu) = \chi_{\Lambda_n^\varphi(\mu)}(\lambda)\check{g}(\lambda, \mu)$$

for $g \in \mathfrak{H}$. Thus, we have

$$\begin{aligned} -2\pi i\, P_1(\Lambda_n) T_2^* &= W_{2,-}^*(n) W_{2,-} - W_{2,-}^*(n) W_{2,+} \\ &= \operatorname*{s-lim}_{\delta \to +0} \operatorname*{w-lim}_{\epsilon \to +0} W_{2,-}^*(\epsilon, n)\big(W_{2,-}(\delta) - W_{2,+}(\delta)\big). \end{aligned} \tag{5.13}$$

Recall the relation (5.5)

$$W_{2,\pm}(\epsilon, n) = \int_{\mathbb{R}} (1 - (K_{2,n} - \nu \pm i\epsilon)^{-1} V_1) P_1(\Lambda_n) \mathrm{d}E_0^{ac}(\nu).$$

We also use

$$W_{2,\pm}(\delta) = \int_{\mathbb{R}} \mathrm{d}E_{K_2}(\nu)(1 - V_1(K_1 - \nu \pm i\delta)^{-1}).$$

For $\check{f} \in \mathfrak{H}_{\Phi_{K_1}}$ we consider

$$\begin{aligned} &\lim_{\epsilon \to +0} \Big(\Phi_{K_1} W_{2,-}^*(\epsilon, n)\big(W_{2,-}(\delta) - W_{2,+}(\delta)\big)\Phi_{K_1}^* \check{f}\Big)(\lambda) \\ &\quad = \lim_{\epsilon \to +0} \Big(\Phi_{K_1} \mathcal{M}(E_{K_1(\mu)}(\Lambda_n^\varphi(\mu)) \int_{\mathbb{R}} \mathrm{d}E_{K_1}(\nu)(1 - V_2(K_{2,n} - \nu + i\epsilon)^{-1}) \\ &\qquad \times \int_{\mathbb{R}} \mathrm{d}E_{K_2}(\eta)\big(1 + V_2(K_1 - \eta + i\delta)^{-1} - 1 - V_2(K_1 - \eta - i\delta)^{-1}\big)\Phi_{K_1}^* \check{f}\Big)(\lambda) \\ &\quad = \lim_{\epsilon \to +0} \Big(\Phi_{K_1} \mathcal{M}(E_{K_1(\mu)}(\Lambda_n^\varphi(\mu)) \int_{\mathbb{R}} \mathrm{d}E_{K_1}(\nu)(1 - V_2(K_{2,n} - \nu + i\epsilon)^{-1}) \\ &\qquad \times \int_{\mathbb{R}} \big((\xi - \nu + i\delta)^{-1} - (\xi - \nu - i\delta)^{-1}\big) V_2 \mathrm{d}E_{K_1}(\xi)\Phi_{K_1}^* \check{f}\Big)(\lambda), \end{aligned}$$

where we used Lemma A.2.19. It follows that

$$\begin{aligned}
&\lim_{\epsilon\to+0}\Big(\Phi_{K_1}W_{2,-}^*(\epsilon,n)\big(W_{2,-}(\delta)-W_{2,+}(\delta)\big)\Phi_{K_1}^*\check{f}\Big)(\lambda)\\
&\quad=\lim_{\epsilon\to+0}\Big(\Phi_{K_1}\mathcal{M}(E_{K_1(\mu)}(\Lambda_n^\varphi(\mu))\int_{\mathbb{R}}\mathrm{d}E_{K_1}(\nu)C_2J_{2,n}(\nu-i\epsilon)\\
&\qquad\qquad\times\int_{\mathbb{R}}\tfrac{-2i\delta}{(\xi-\nu)^2+\delta^2}C_2\mathrm{d}E_{K_1}(\xi)\Phi_{K_1}^*\check{f}\Big)(\lambda)\\
&\quad=\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\sqrt{Y_2(\lambda)}J_{2,n}(\lambda-i0)\int_{\mathbb{R}}\mathrm{d}\xi\tfrac{-2i\delta}{(\xi-\nu)^2+\delta^2}\sqrt{Y_2(\xi)}\check{f}(\xi)
\end{aligned}$$

for *a.e.* $\lambda\in\mathbb{R}$, where the limit $J_{2,n}(\lambda-i0)$ exists in the Hilbert-Schmidt norm for a.e. $\lambda\in\mathbb{R}$ since $C_2\in\mathfrak{L}_2(\mathfrak{H})$. Taking the limit $\delta\to+0$ and using Lemma A.2.20, we obtain

$$\begin{aligned}
&\lim_{\delta\to+0}\lim_{\epsilon\to+0}\Big(\Phi_{K_1}W_{2,-}^*(\epsilon,n)\big(W_{2,-}(\delta)-W_{2,+}(\delta)\big)\Phi_{K_1}^*\check{f}\Big)(\lambda)\\
&\quad=-2\pi i\,\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\sqrt{Y_2(\lambda)}J_{2,n}(\lambda-i0)\sqrt{Y_2(\lambda)}\check{f}(\lambda).
\end{aligned}$$

Since

$$(\Phi_{K_1}\mathcal{M}(E_{K_1(\mu)}(\Lambda_n^\varphi(\mu))T_2^*f)(\lambda)=\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\check{T}_2^*(\lambda),$$

the lemma follows from (5.13). □

Using Lemma 5.2.7, we can derive a similar formula for the transition matrix $\check{T}_1(\lambda)$, $\lambda\in\mathbb{R}$, but the formula holds only in the fiber.

Proposition 5.2.9. *For a.e. $\lambda\in\mathbb{R}$ the transition matrix $\check{T}_1(\lambda)$ for $W_{1,\pm}$ with respect to Φ_{K_0} is a multiplication operator on $\mathfrak{H}_\lambda=L^2(\mathbb{R}_+^0,\mathrm{d}\mathfrak{m}(\mu),\mathfrak{h}_\lambda(\mu))$ and satisfies*

$$\chi_{\Lambda_n(\mu)}(\lambda)\check{T}_1(\lambda,\mu)=\chi_{\Lambda_n(\mu)}(\lambda)\sqrt{Y_1(\lambda,\mu)}J_{1,n}(\lambda+i0,\mu)\sqrt{Y_1(\lambda,\mu)}$$

for a.e. $\lambda\in\mathbb{R}$ and $\mathfrak{m}$-a.e. $\mu\geq0$, where

$$J_{1,n}(\lambda+i0,\mu)=\lim_{\epsilon\to+0}Z_1(\mu)-Z_1(\mu)C_1(\mu)(K_{1,n}(\mu)-\lambda-i\epsilon)^{-1}C_1^*(\mu)Z_1(\mu)$$

and the limit is taken in the Hilbert-Schmidt norm.

Proof. The proof is also almost identical to the proof of Proposition 5.2.8, except that we have to work in the fiber. Note that $W_{1,\pm}(n)=W_{1,\pm}P_0(\Lambda_n)$ and

$$(\Phi_0P_0(\Lambda_n)g)(\lambda,\mu)=(\Phi_0\mathcal{M}(E_{K_0(\mu)}(\Lambda_n^\varphi(\mu)))g)(\lambda,\mu)=\chi_{\Lambda_n^\varphi(\mu)}(\lambda)\widehat{g}(\lambda,\mu)$$

for $g\in\mathfrak{H}_0^{ac}$. Thus, we have

$$\begin{aligned}
-2\pi iP_0(\Lambda_n)T_1^*&=W_{1,-}^*(n)W_{1,-}-W_{1,-}^*(n)W_{1,+}\\
&=\operatorname*{s-lim}_{\delta\to+0}\operatorname*{w-lim}_{\epsilon\to+0}W_{1,-}^*(\epsilon,n)\big(W_{1,-}(\delta)-W_{1,+}(\delta)\big).
\end{aligned}\tag{5.14}$$

Recall the relation (5.4)

$$W_{1,\pm}(\epsilon,n)=\int_{\mathbb{R}}(1-(K_{1,n}-\nu\pm i\epsilon)^{-1}V_1)P_0(\Lambda_n)\mathrm{d}E_0^{ac}(\nu).$$

We also use

$$W_{1,\pm}(\delta)=\int_{\mathbb{R}}\mathrm{d}E_{K_1}(\nu)(1-V_1(K_0-\nu\pm i\delta)^{-1})P_0^{ac}.$$

For $\check{f}\in\mathfrak{H}_{\Phi_{K_0}}$ we consider

$$\begin{aligned}
&\lim_{\epsilon\to+0}\Big(\Phi_{K_0}W_{1,-}^*(\epsilon,n)(W_{1,-}(\delta)-W_{1,+}(\delta))\Phi_{K_0}^*\check{f}\Big)(\lambda)\\
&\quad=\lim_{\epsilon\to+0}\Big(\Phi_{K_0}P_0(\Lambda_n)\int_{\mathbb{R}}\mathrm{d}E_0^{ac}(\nu)(1-V_1^*(K_{1,n}-\nu+i\epsilon)^{-1})\int_{\mathbb{R}}\mathrm{d}E_{K_1}(\eta)\\
&\qquad\qquad\times\big(1+V_1(K_0-\eta+i\delta)^{-1}-1-V_1(K_0-\eta-i\delta)^{-1}\big)\Phi_{K_0}^*\check{f}\Big)(\lambda)\\
&\quad=\lim_{\epsilon\to+0}\Big(\Phi_{K_0}P_0(\Lambda_n)\int_{\mathbb{R}}\mathrm{d}E_0^{ac}(\nu)(1-V_1(K_{1,n}-\nu+i\epsilon)^{-1})\\
&\qquad\qquad\times\int_{\mathbb{R}}\big((\xi-\nu+i\delta)^{-1}-(\xi-\nu-i\delta)^{-1}\big)V_1\mathrm{d}E_0^{ac}(\xi)\Phi_{K_0}^*\check{f}\Big)(\lambda),
\end{aligned}$$

where we used Lemma A.2.19. Since $K_1=\mathcal{M}(K_1(\mu))$ and $V_1=\mathcal{M}(C_1^*(\mu)Z_1(\mu)C_1(\mu))$, we can use Lemma 3.1.5, which describes the action of $\Phi_{K_0}(\mu)$, to obtain

$$\begin{aligned}
&\lim_{\epsilon\to+0}\Big(\Phi_{K_0}W_{1,-}^*(\epsilon,n)(W_{1,-}(\delta)-W_{1,+}(\delta))\Phi_{K_0}^*\check{f}\Big)(\lambda,\mu)\\
&\quad=\lim_{\epsilon\to+0}\Big(\Phi_{K_0}\mathcal{M}(E_{K_0(\mu)}(\Lambda_n^{\varphi}(\mu))\int_{\mathbb{R}}\mathrm{d}E_0^{ac}(\nu)C_1^*(Z_1-Z_1C_1(K_{1,n}-\nu+i\epsilon)^{-1}C_1^*Z_1)\\
&\qquad\qquad\times\int_{\mathbb{R}}\tfrac{-2i\delta}{(\xi-\nu)^2+\delta^2}C_1\mathrm{d}E_0^{ac}(\xi)\Phi_{K_0}^*\check{f}\Big)(\lambda,\mu)\\
&\quad=\lim_{\epsilon\to+0}\chi_{\Lambda_n^{\varphi}(\mu)}(\lambda)\sqrt{Y_1(\lambda,\mu)}(Z_1(\mu)-Z_1(\mu)C_1(\mu)(K_{1,n}(\mu)-\lambda+i\epsilon)^{-1}C_1^*(\mu)Z_1(\mu))\\
&\qquad\qquad\times\int_{\mathbb{R}}\tfrac{-2i\delta}{(\xi-\nu)^2+\delta^2}C_1(\mu)\mathrm{d}E_{K_0(\mu)}^{ac}(\xi)\Phi_{K_0(\mu)}^*\check{f}(\cdot,\mu)\\
&\quad=\chi_{\Lambda_n^{\varphi}(\mu)}(\lambda)\sqrt{Y_1(\lambda,\mu)}J_{1,n}(\lambda-i0,\mu)\int_{\mathbb{R}}\mathrm{d}\xi\,\tfrac{-2i\delta}{(\xi-\nu)^2+\delta^2}\sqrt{Y_1(\xi,\mu)}\check{f}(\xi,\mu)
\end{aligned}$$

for *a.e.* $\lambda\in\mathbb{R}$, $\mathfrak{m}$-a.e. $\mu\geq 0$, where the limit $J_{1,n}(\lambda-i0,\mu)$ exists in the Hilbert-Schmidt norm on $\mathfrak{h}$ since $C_1(\mu)\in\mathfrak{L}_2(\mathfrak{h})$. Taking the limit $\delta\to+0$ and using Lemma A.2.20, we arrive at

$$\begin{aligned}
&\lim_{\delta\to+0}\lim_{\epsilon\to+0}\Big(\Phi_{K_0}W_{1,-}^*(\epsilon,n)(W_{1,-}(\epsilon)-W_{1,+}(\epsilon))\Phi_{K_0}^*\check{f}\Big)(\lambda,\mu)\\
&\qquad=-2\pi i\chi_{\Lambda_n^{\varphi}(\mu)}(\lambda)\sqrt{Y_1(\lambda,\mu)}J_{1,n}(\lambda-i0,\mu)\sqrt{Y_1(\lambda,\mu)}\check{f}(\lambda,\mu).
\end{aligned}$$

Since

$$(\Phi_{K_0}P_0(\Lambda_n)T_1^*f)(\lambda,\mu)=\chi_{\Lambda_n^{\varphi}(\mu)}(\lambda)\check{T}_1^*(\lambda,\mu),$$

the proposition follows from (5.14). □

5.2.3 Calculation of the Landauer-Büttiker formula

With the smoothness, the spectral representations Φ_{K_0} and Φ_{K_1}, and the formulae for $\check{T}_1(\lambda)$ and $\check{T}_2(\lambda)$, $\lambda \in \mathbb{R}$, we now possess the essential ingredients for the proof of the Landauer-Büttiker formula of Theorem 5.1.8. Recall that we want to show

$$\begin{aligned}\mathfrak{J}_Q &= \lim_{n\to\infty}\lim_{\epsilon\to+0} -2\,\Im\mathrm{m}\big[\mathrm{Tr}\big(\varrho_0 W_{1,-}^*(n)W_{2,-}^*(\epsilon,n)(V_1+V_2)Q_nW_{2,-}(\epsilon,n)W_{1,-}(n)\big)\big]\\ &= -2\pi\int_{\mathbb{R}}\mathrm{d}\lambda\mathrm{Tr}\Big(\rho(\lambda)\big(T^*(\lambda)T(\lambda)Q(\lambda)-T^*(\lambda)Q(\lambda)T(\lambda)\big)+(2\pi i)^{-1}T(\lambda)[Q(\lambda),\rho(\lambda)]\Big)\\ &= -2\int_{\mathbb{R}}\mathrm{d}\lambda\,\mathrm{Tr}\Big(\Im\mathrm{m}[\rho(\lambda)T^*(\lambda)Q(\lambda)]-\pi\rho(\lambda)T^*(\lambda)Q(\lambda)T(\lambda)\Big),\end{aligned}$$

where we used $T^*-T=2\pi i\,T^*T$ in the last equality. In this equation, $T(\lambda)$ is taken with respect to a spectral representation Φ_{H_0} of H_0^{ac}. But we want to work with K_0 and hence represent $\mathfrak{J}_Q$ using $\check{T}(\lambda)$, taken with respect to the spectral representation Φ_{K_0} of K_0^{ac}. Note that we obtain from Lemma 3.1.11 that if Φ_{H_0} is a spectral representation of H_0^{ac}, then $\Psi_\varphi\Phi_{H_0}$ is a spectral representation of K_0^{ac} with

$$\check{g}(\lambda)=(\Psi_\varphi\widehat{g})(\lambda)=-\lambda\,\widehat{g}(\varphi^{-1}(\lambda)),\qquad \varphi^{-1}(\lambda)=-\lambda^{-1}-1.$$

We already used the connection between H_0 and K_0 in the proof of the Landauer-Büttiker formula in Chapter 3. Recall that

$$\Psi_\varphi\mathcal{M}(X(\lambda))\Psi_\varphi^*=\mathcal{M}\big(X(\varphi^{-1}(\lambda))\big).$$

Further note that $\rho(\lambda)=(\lambda+1)^{-2}\varrho_0(\lambda)=\varphi(\lambda)^2\varrho_0(\lambda)$ and $\frac{\mathrm{d}}{\mathrm{d}\nu}\varphi^{-1}(\nu)=\nu^{-2}$. Hence,

$$\begin{aligned}&\int_{\mathbb{R}}\mathrm{d}\lambda\,\mathrm{Tr}\Big(\Im\mathrm{m}[\rho(\lambda)T^*(\lambda)Q(\lambda)]-\pi\rho(\lambda)T^*(\lambda)Q(\lambda)T(\lambda)\Big)\\ &\quad=\int_{\mathbb{R}}\mathrm{d}\nu\,\nu^2\nu^{-2}\mathrm{Tr}\Big(\Im\mathrm{m}[\varrho_0(\varphi^{-1}(\nu))T^*(\varphi^{-1}(\nu))Q(\varphi^{-1}(\nu))]\\ &\qquad\qquad-\pi\varrho_0(\varphi^{-1}(\nu))T^*(\varphi^{-1}(\nu))Q(\varphi^{-1}(\nu))T(\varphi^{-1}(\nu))\Big)\\ &\quad=\int_{\mathbb{R}}\mathrm{d}\nu\,\mathrm{Tr}\Big(\Im\mathrm{m}[\check{\varrho}_0(\nu)\check{T}^*(\nu)\check{Q}(\nu)]-\pi\check{\varrho}_0(\nu)\check{T}^*(\nu)\check{Q}(\nu)\check{T}(\nu)\Big).\end{aligned}$$

Thus, it suffices to prove

$$\begin{aligned}\mathfrak{J}_Q &= \lim_{n\to\infty}\lim_{\epsilon\to+0} 2\,\Im\mathrm{m}\big[\mathrm{Tr}\big(\varrho_0 W_{1,-}^*(n)W_{2,-}^*(\epsilon,n)(V_1+V_2)Q_nW_{2,-}(\epsilon,n)W_{1,-}(n)\big)\big]\\ &= -2\int_{\mathbb{R}}\mathrm{d}\lambda\,\mathrm{Tr}\Big(\Im\mathrm{m}[\check{\varrho}_0(\lambda)\check{T}^*(\lambda)\check{Q}(\lambda)]-\pi\check{\varrho}_0(\lambda)\check{T}^*(\lambda)\check{Q}(\lambda)\check{T}(\lambda)\Big).\end{aligned}\tag{5.15}$$

Recall that $W_{1,\pm}(n)=\text{s-lim}_{\epsilon\to+0}W_{1,\pm}(\epsilon,n)$ with

$$\begin{aligned}W_{1,\pm}(\epsilon,n)&=\int_{\mathbb{R}}(1-(K_{1,n}-\lambda\pm i\epsilon)^{-1}V_1)P_0(\Lambda_n)\mathrm{d}E_0^{ac}(\lambda)\\ &=\int_{\mathbb{R}}\mathrm{d}E_{K_1}(\lambda)P_1(\Lambda_n)(1-V_1(K_{0,n}-\lambda\pm i\epsilon)^{-1})P_0^{ac}\end{aligned}$$

and

$$\begin{aligned} W_{2,\pm}(\epsilon,n) &= \int_{\mathbb{R}} (1-(K_{2,n}-\lambda\pm i\epsilon)^{-1}V_2)P_1(\Lambda_n)\mathrm{d}E_{K_1}(\lambda) \\ &= \int_{\mathbb{R}} \mathrm{d}E_{K_2}(\lambda)P_2(\Lambda_n)(1-V_2(K_{1,n}-\lambda\pm i\epsilon)^{-1}). \end{aligned}$$

Note that the perturbations satisfy $P_1(\Lambda_n)(K_{1,n}-K_{0,n})P_0(\Lambda_n) = P_1(\Lambda_n)V_1P_0(\Lambda_n)$ and $P_2(\Lambda_n)(K_{2,n}-K_{1,n})P_1(\Lambda_n) = P_2(\Lambda_n)V_2P_1(\Lambda_n)$. It follows that

$$\begin{aligned} \widetilde{W}_{1,\pm}(\epsilon,n) &= \int_{\mathbb{R}} (K_{1,n}-\lambda\pm i\epsilon)^{-1}V_1P_0(\Lambda_n)\mathrm{d}E_0^{ac}(\lambda) \\ &= \int_{\mathbb{R}} (K_{0,n}-\lambda\pm i\epsilon)^{-1}(1-V_1(K_{1,n}-\lambda\pm i\epsilon)^{-1})V_1P_0(\Lambda_n)\mathrm{d}E_0^{ac}(\lambda) \end{aligned}$$

and similarly

$$\widetilde{W}_{2,\pm}(\epsilon,n) = \int_{\mathbb{R}} (K_{1,n}-\lambda\pm i\epsilon)^{-1}(1-V_2(K_{2,n}-\lambda\pm i\epsilon)^{-1})V_2P_1(\Lambda_n)\mathrm{d}E_{K_1}(\lambda).$$

For any $\delta > 0$ we get

$$\begin{aligned} &P_{0,n}^{ac}(V_1+V_2)W_{2,-}(\epsilon,n) \\ &= P_{0,n}^{ac}V_1P_1(\Lambda_n) + F(\epsilon,\delta,n) + \int\limits_{\mathbb{R}} \mathrm{d}E_0^{ac}(\lambda)P_{0,n}^{ac}\int\limits_{\mathbb{R}} C_2J_{2,n}(\nu+i\epsilon)C_2P_1(\Lambda_n)\mathrm{d}E_{K_1}(\nu) \\ &\qquad - \int\limits_{\mathbb{R}} \mathrm{d}E_0^{ac}(\lambda)P_{0,n}^{ac}V_1(K_{1,n}-\lambda-i\delta)^{-1}\int\limits_{\mathbb{R}} C_2J_{2,n}(\nu+i\epsilon)C_2P_1(\Lambda_n)\mathrm{d}E_{K_1}(\nu) \\ &= P_{0,n}^{ac}V_1P_1(\Lambda_n) + F(\epsilon,\delta,n) + \int\limits_{\mathbb{R}} \mathrm{d}E_0^{ac}(\lambda)P_{0,n}^{ac}(1-V_1(K_{1,n}-\lambda-i\delta)^{-1})C_2 \\ &\qquad\qquad \times \int\limits_{\mathbb{R}} J_{2,n}(\nu+i\epsilon)C_2P_1(\Lambda_n)\mathrm{d}E_{K_1}(\nu) \\ &= P_{0,n}^{ac}V_1P_1(\Lambda_n) + W_{1,+}^*(\delta,n)V_2W_{2,-}(\epsilon,n) + F(\epsilon,\delta,n), \end{aligned} \tag{5.16}$$

where

$$\begin{aligned} F(\epsilon,\delta,n) &= \int\limits_{\mathbb{R}} \mathrm{d}E_0^{ac}(\lambda)P_{0,n}^{ac}V_1(K_{1,n}-\lambda-i\delta)^{-1}\int\limits_{\mathbb{R}} C_2J_{2,n}(\nu+i\epsilon)C_2P_1(\Lambda_n)\mathrm{d}E_{K_1}(\nu) \\ &\quad - \int\limits_{\mathbb{R}} \mathrm{d}E_0^{ac}(\lambda)P_{0,n}^{ac}\int\limits_{\mathbb{R}} V_1(K_{1,n}-\nu-i\epsilon)^{-1}C_2J_{2,n}(\nu+i\epsilon)C_2P_1(\Lambda_n)\mathrm{d}E_{K_1}(\nu) \end{aligned} \tag{5.17}$$

is trace class by Lemma A.2.17. For the argument of the trace in the definition of the flux (5.8), we have

$$\begin{aligned} &W_{1,-}^*(n)W_{2,-}^*(\epsilon,n)(V_1+V_2)Q_nW_{2,-}(\epsilon,n)W_{1,-}(n) \\ &\quad = W_{1,-}^*(n)\big(V_1P_{0,n}^{ac} + W_{2,-}^*(\epsilon,n)V_2W_{1,+}(\delta,n) + F^*(\epsilon,\delta,n)\big)Q_nW_{2,-}(\epsilon,n)W_{1,-}(n). \end{aligned}$$

Thus,

$$\begin{aligned}
&W_{1,-}^*(n)W_{2,-}^*(\epsilon,n)(V_1+V_2)Q_nW_{2,-}(\epsilon,n)W_{1,-}(n)\\
&\quad= W_{1,-}^*(n)V_1P_{0,n}^{ac}Q_nW_{1,-}(n)\\
&\qquad+ W_{1,-}^*(n)\big(W_{2,-}^*(\epsilon,n)V_2W_{1,+}(\delta,n)+F(\epsilon,\delta,n)\big)Q_n\\
&\qquad- W_{1,-}^*(n)V_1P_{0,n}^{ac}Q_n\widetilde{W}_{2,-}(\epsilon,n)W_{1,-}(n)\\
&\qquad- W_{1,-}^*(n)\big(W_{2,-}^*(\epsilon,n)V_2W_{1,+}(\delta,n)+F^*(\epsilon,\delta,n)\big)Q_n\widetilde{W}_{1,-}(n)\\
&\qquad- W_{1,-}^*(n)\big(W_{2,-}^*(\epsilon,n)V_2W_{1,+}(\delta,n)+F^*(\epsilon,\delta,n)\big)Q_n\widetilde{W}_{2,-}(\epsilon,n)W_{1,-}(n)
\end{aligned}$$

for any $\delta>0$, using $W_{1,-}^*(n)P_1(\Lambda_n)=W_{1,-}^*(n)$. We introduce the shorthand notation

$$\begin{aligned}
\Sigma_1(n)&=W_{1,-}^*(n)V_1P_{0,n}^{ac}Q_nW_{1,-}(n),\\
\Sigma_2(\epsilon,\delta,n)&=W_{1,-}^*(n)\big(W_{2,-}^*(\epsilon,n)V_2W_{1,+}(\delta,n)+F(\epsilon,\delta,n)\big)Q_n,\\
\Sigma_3(\epsilon,\delta,n)&=-W_{1,-}^*(n)V_1P_{0,n}^{ac}Q_n\widetilde{W}_{2,-}(\epsilon,n)W_{1,-}(n)\\
&\qquad- W_{1,-}^*(n)\big(W_{2,-}^*(\epsilon,n)V_2W_{1,+}(\delta,n)+F^*(\epsilon,\delta,n)\big)Q_n\widetilde{W}_{1,-}(n),\\
\Sigma_4(\epsilon,\delta,n)&=-W_{1,-}^*(n)\big(W_{2,-}^*(\epsilon,n)V_2W_{1,+}(\delta,n)+F^*(\epsilon,\delta,n)\big)\\
&\qquad\qquad\times Q_n\widetilde{W}_{2,-}(\epsilon,n)W_{1,-}(n).
\end{aligned}$$

Hence, by (5.16)

$$\begin{aligned}
&W_{1,-}^*(n)W_{2,-}^*(\epsilon,n)(V_1+V_2)Q_nW_{2,-}(\epsilon,n)W_{1,-}(n)\\
&\qquad\qquad=\Sigma_1(n)+\Sigma_2(\epsilon,\delta,n)+\Sigma_3(\epsilon,\delta,n)+\Sigma_4(\epsilon,\delta,n).
\end{aligned}$$

Since this holds for all $\delta>0$, we may write

$$\mathfrak{J}_Q=\lim_{n\to\infty}\lim_{\epsilon\to+0}\lim_{\delta\to+0}-2\,\Im\mathrm{m}\big[\mathrm{Tr}\big(\varrho_0(\Sigma_1(n)+\Sigma_2(\epsilon,\delta,n)+\Sigma_3(\epsilon,\delta,n)+\Sigma_4(\epsilon,\delta,n))\big)\big],\tag{5.18}$$

were $\varrho_0\Sigma_1(n)$ and $\Sigma_j(\epsilon,\delta,n)$, $j\in\{2,3,4\}$, are trace class. Let us give a sketch of the proof that follows. The Landauer-Büttiker formula (5.15) contains the two terms

$$\Im\mathrm{m}[\check{\varrho}_0(\lambda)\check{T}^*(\lambda)\check{Q}(\lambda)]\qquad\text{and}\qquad\pi\check{\varrho}_0(\lambda)\check{T}^*(\lambda)\check{Q}(\lambda)\check{T}(\lambda).$$

Since $\check{T}(\lambda)=\check{T}_1(\lambda)+\check{W}_{1,+}^*(\lambda)\check{T}_2(\lambda)\check{W}_{1,-}(\lambda)$, we expect summands of the type

$$\Im\mathrm{m}[\check{\varrho}_0(\lambda)\check{T}_1^*(\lambda)\check{Q}(\lambda)]+\pi\check{\varrho}_0(\lambda)\check{T}_1^*(\lambda)\check{Q}(\lambda)\check{T}_1(\lambda),\tag{5.19}$$

as well as

$$\begin{aligned}
&\Im\mathrm{m}\big[\check{\varrho}_0(\lambda)\check{W}_{1,-}^*(\lambda)\check{T}_2^*(\lambda)\check{W}_{1,+}(\lambda)\check{Q}(\lambda)\big]\\
&\qquad+\pi\check{\varrho}_0(\lambda)\check{W}_{1,-}^*(\lambda)\check{T}_2^*(\lambda)\check{W}_{1,+}(\lambda)\check{Q}(\lambda)\check{W}_{1,+}^*(\lambda)\check{T}_2(\lambda)\check{W}_{1,-}(\lambda)
\end{aligned}\tag{5.20}$$

and the mixed terms

$$\pi\check{T}_1^*(\lambda)\check{Q}(\lambda)\check{W}_{1,+}^*(\lambda)\check{T}_2(\lambda)\check{W}_{1,-}(\lambda)+\pi\check{W}_{1,-}^*(\lambda)\check{T}_2^*(\lambda)\check{W}_{1,+}(\lambda)\check{Q}(\lambda)\check{T}_1(\lambda)\tag{5.21}$$

to appear. It will turn out that Σ_1 corresponds to (5.19), Σ_2 corresponds to the first, Σ_4 to the second summand of (5.20), and Σ_3 corresponds to the mixed terms (5.21). Roughly speaking, $W_{j,-}^*(\epsilon)V_j$ gives us T_j^* and $\widetilde{W}_{j,-}(\epsilon)$ gives us T_j with an approximation of the delta function, $j \in \{1,2\}$. We proceed by calculating these contributions.

In the following we make use of the fact that the spectral representation Φ_{K_0} maps a multiplication operator $\mathcal{M}(X(\mu))$ on $L^2(\mathbb{R}^0_+, \mathrm{d}\mathfrak{m}(\mu), \mathfrak{h})$ onto a family of multiplication operators $\mathcal{M}(\check{X}(\lambda,\mu))$ on $L^2(\mathbb{R}^0_+, \mathrm{d}\mathfrak{m}(\mu), \mathfrak{h}_\lambda(\mu))$. In particular, $\check{\varrho}_0(\lambda,\mu) = \check{\varrho}_0(\lambda,\mu)\delta(\mu)$ by Assumption (A3). This relation implies that only the fiber $\mu = 0$ is relevant in the following lemma since Σ_1 is in fact a multiplication operator on $L^2(\mathbb{R}^0_+, \mathrm{d}\mathfrak{m}(\mu), \mathfrak{h})$.

Lemma 5.2.10. *We have*

$$\begin{aligned}&\lim_{n\to\infty} \Im\mathrm{m}\big[\mathrm{Tr}\big(\varrho_0\Sigma_1(n)\big)\big]\\ &\qquad = \int_{\mathbb{R}} \mathrm{d}\lambda \mathrm{Tr}\Big(\Im\mathrm{m}[\check{\varrho}_0(\lambda)\check{T}_1^*(\lambda)\check{Q}(\lambda)] - \pi\check{\varrho}_0(\lambda)\check{T}_1^*(\lambda)\check{Q}(\lambda)\check{T}_1(\lambda)\Big).\end{aligned} \tag{5.22}$$

Proof. Since $W_{1,-}(\epsilon,n)$ is in fact a multiplication operator on $L^2(\mathbb{R}^0_+, \mathrm{d}\mathfrak{m}(\mu), \mathfrak{h})$ and $\rho(\mu) = \rho_0\,\delta(\mu)$, we get that

$$\varrho_0\Sigma_1(n) = \lim_{\delta\to+0}\lim_{\epsilon\to+0} \varrho_0 W_{1,-}^*(\epsilon,n)V_1P_{0,n}^{ac}Q_n - \varrho_0 W_{1,-}^*(\epsilon,n)V_1P_{0,n}^{ac}Q_n\widetilde{W}_{1,-}(\delta,n)$$

is trace class, where the limits are taken in the trace norm. Recall that the projection $P_0(\Lambda_n)$ satisfies $(\Phi_0 P_0(\Lambda_n)g)(\lambda,\mu) = \chi_{\Lambda_n^\varphi(\mu)}(\lambda)\check{g}(\lambda,\mu)$. Thus, we can use Lemma 5.2.7 to obtain

$$\begin{aligned}&\big(\Phi_{K_0}W_{1,-}^*(\epsilon,n)V_1P_{0,n}^{ac}g\big)(\lambda,\mu)\\ &\quad= \Big(\Phi_{K_0}P_0(\Lambda_n)\int_{\mathbb{R}} \mathrm{d}E_0^{ac}(\nu)C_1^*J_{1,n}(\nu-i\epsilon)\int_{\mathbb{R}} C_1\mathrm{d}E_0^{ac}(\eta)P_0(\Lambda_n)\Phi_{K_0}^*\check{g}\Big)(\lambda,\mu)\\ &\quad= \chi_{\Lambda_n^\varphi(\mu)}(\lambda)\sqrt{Y_1(\lambda,\mu)}J_{1,n}(\lambda-i\epsilon,\mu)\int_{\Lambda_n}\mathrm{d}\eta\sqrt{Y_1(\eta,\mu)}\check{g}(\eta,\mu)\end{aligned}$$

for $g \in \mathfrak{H}_0^{ac}$. The limit $J_{1,n}(\lambda - i0,\mu)$ exists in the Hilbert-Schmidt norm for $\mathfrak{m}$-a.e. $\mu \geq 0$ and a.e. $\lambda \in \mathbb{R}$. We get

$$\begin{aligned}&\mathrm{Tr}\big(\varrho_0 W_{1,-}^*(n)V_1P_{0,n}^{ac}Q_n\big)\\ &\quad= \int_{\mathbb{R}}\mathrm{d}\lambda\,\chi_{\Lambda_n^\varphi(0)}(\lambda)\mathrm{Tr}\Big(\check{\varrho}_0(\lambda,0)\sqrt{Y_1(\lambda,0)}J_{1,n}(\lambda-i0,0)\sqrt{Y_1(\lambda,0)}\check{Q}(\lambda,0)\Big)\\ &\quad= \int_{\mathbb{R}}\mathrm{d}\lambda\,\chi_{\Lambda_n^\varphi(0)}(\lambda)\mathrm{Tr}\big(\check{\varrho}_0(\lambda,0)\check{T}_1^*(\lambda,0)\check{Q}(\lambda,0)\big).\end{aligned} \tag{5.23}$$

For the second part of Σ_1, we obtain

$$\begin{aligned}&W_{1,-}^*(\epsilon,n)V_1P_{0,n}^{ac}Q_n\widetilde{W}_{1,-}(\delta,n)\\ &= P_0(\Lambda_n)\int_{\mathbb{R}}\mathrm{d}E_0^{ac}(\nu)\big(1 - V_1(K_{1,n}-\nu+i\epsilon)^{-1}\big)V_1Q_n\\ &\qquad\qquad\times\int_{\mathbb{R}}(K_{1,n}-\eta-i\delta)^{-1}V_1\mathrm{d}E_0^{ac}(\eta)P_0(\Lambda_n).\end{aligned}$$

Thus,

$$\begin{aligned}
&W^*_{1,-}(\epsilon,n)V_1P^{ac}_{0,n}Q_n\widetilde{W}_{1,-}(\delta,n)\\
&= P_0(\Lambda_n)\int_{\mathbb{R}}\mathrm{d}E^{ac}_0(\nu)C_1^*J_{1,n}(\nu-i\epsilon)C_1Q_n\\
&\qquad\times\int_{\mathbb{R}}(K_{0,n}-\eta-i\delta)^{-1}C_1^*J_{1,n}(\eta+i\delta)C_1\mathrm{d}E^{ac}_0(\eta)P_0(\Lambda_n).
\end{aligned}$$

Hence, by Lemma 5.2.7

$$\begin{aligned}
&\big(\Phi_{K_0}W^*_{1,-}(\epsilon,n)V_1Q_n\widetilde{W}_{1,-}(\delta,n)\Phi^*_{K_0}\check{g}\big)(\lambda,\mu)\\
&=\chi_{\Lambda^\varphi_n(\mu)}(\lambda)\sqrt{Y_1(\lambda,\mu)}J_{1,n}(\lambda-i\epsilon,\mu)C_1(\mu)Q_n(\mu)\\
&\qquad\times\int_{\mathbb{R}}\mathrm{d}\eta\,(K_{0,n}(\mu)-\eta-i\delta)^{-1}C_1^*(\mu)J_{1,n}(\eta+i\delta,\mu)\sqrt{Y_1(\eta,\mu)}\check{g}(\eta,\mu).
\end{aligned}$$

We can once more use Lemma 5.2.7 to obtain

$$\begin{aligned}
&\big(\Phi_{K_0}W^*_{1,-}(\epsilon,n)V_1Q_n\widetilde{W}_{1,-}(\delta,n)\Phi^*_{K_0}\check{g}\big)(\lambda,\mu)\\
&\quad=\chi_{\Lambda^\varphi_n(\mu)}(\lambda)\sqrt{Y_1(\lambda,\mu)}J_{1,n}(\lambda-i\epsilon,\mu)\int_{\mathbb{R}}C_1(\mu)\mathrm{d}E^{ac}_{K_0(\mu)}(\nu)Q_n(\mu)\\
&\qquad\times\int_{\mathbb{R}}\mathrm{d}\eta\int_{\mathbb{R}}\mathrm{d}E^{ac}_{K_0(\mu)}(\xi)C_1^*(\mu)(\xi-\eta-i\delta)^{-1}J_{1,n}(\eta+i\delta,\mu)\sqrt{Y_1(\eta,\mu)}\check{g}(\eta,\mu)\\
&\quad=\chi_{\Lambda^\varphi_n(\mu)}(\lambda)\sqrt{Y_1(\lambda,\mu)}J_{1,n}(\lambda-i\epsilon,\mu)\int_{\mathbb{R}}\mathrm{d}\nu\sqrt{Y_1(\nu,\mu)}\chi_{\Lambda^\varphi_n(\mu)}(\nu)\check{Q}(\nu,\mu)\\
&\qquad\qquad\times\int_{\mathbb{R}}\mathrm{d}\eta\,\sqrt{Y_1(\nu,\mu)}(\nu-\eta-i\delta)^{-1}J_{1,n}(\eta+i\delta,\mu)\sqrt{Y_1(\eta,\mu)}\check{g}(\eta,\mu).
\end{aligned}$$

Note that $\Lambda^\varphi_n(\mu)\subset\Lambda^\varphi_n$. Also, $J_{1,n}(\lambda\pm i\delta,\mu)$ and

$$\int_{\mathbb{R}}\mathrm{d}\nu\sqrt{Y_1(\nu,\mu)}\chi_{\Lambda^\varphi_n(\mu)}(\nu)\check{Q}(\nu,\mu)\sqrt{Y_1(\nu,\mu)}(\nu-\lambda-i\delta)^{-1}$$

converge uniformly for a.e. $\lambda\in\Lambda^\varphi_n$ as $\delta\to+0$. Thus, including ϱ_0 and taking the trace leads to

$$\begin{aligned}
&\lim_{\delta\to+0}\lim_{\epsilon\to+0}\mathrm{Tr}\big(\Phi_{K_0}\varrho_0W^*_{1,-}(\epsilon,n)V_1P^{ac}_{0,n}Q_n\widetilde{W}_{1,-}(\delta,n)\Phi^*_{K_0}\big)\\
&\quad=\lim_{\delta\to+0}\int_{\mathbb{R}}\mathrm{d}\lambda\,\chi_{\Lambda^\varphi_n(0)}(\lambda)\mathrm{Tr}\Big(\check{\varrho}_0(\lambda,0)\sqrt{Y_1(\lambda,0)}J_{1,n}(\lambda-i0,0)\int_{\mathbb{R}}\mathrm{d}\nu\,\sqrt{Y_1(\nu,0)}\check{Q}(\nu,0)\\
&\qquad\qquad\times\chi_{\Lambda^\varphi_n(0)}(\nu)\sqrt{Y_1(\nu,0)}(\nu-\lambda-i\delta)^{-1}J_1(\lambda+i0,0)\sqrt{Y_1(\lambda,0)}\Big).
\end{aligned}$$

We take the imaginary part and obtain

$$\begin{aligned}
&\lim_{\delta\to+0}\lim_{\epsilon\to+0}\Im\mathrm{m}\big[\mathrm{Tr}\big(\varrho_0W^*_{1,-}(\epsilon,n)V_1P^{ac}_{0,n}Q_n\widetilde{W}_{1,-}(\delta,n)\big)\big]\\
&\quad=\lim_{\delta\to+0}\int_{\mathbb{R}}\mathrm{d}\lambda\,\chi_{\Lambda^\varphi_n(0)}(\lambda)\mathrm{Tr}\Big(\check{\varrho}_0(\lambda,0)\sqrt{Y_1(\lambda,0)}J_{1,n}(\lambda-i0,0)\int_{\mathbb{R}}\mathrm{d}\nu\sqrt{Y_1(\nu,0)}\check{Q}(\nu,0)\\
&\qquad\qquad\times\chi_{\Lambda^\varphi_n(0)}(\nu)\sqrt{Y_1(\nu,0)}\tfrac{\delta}{(\nu-\lambda)^2+\delta^2}J_1(\lambda+i0,0)\sqrt{Y_1(\lambda,0)}\Big)
\end{aligned}$$

The limit exists by Lemma A.2.20, whence

$$\begin{aligned}\lim_{\delta\to+0}\lim_{\epsilon\to+0}\Im\mathrm{m}\big[\mathrm{Tr}\big(\varrho_0 W_{1,-}^*(\epsilon,n)V_1P_{0,n}^{ac}Q_n\widetilde{W}_{1,-}(\delta,n)\big)\big]\\ =\pi\int_{\mathbb{R}}\mathrm{d}\lambda\,\chi_{\Lambda_n^\varphi(0)}(\lambda)\mathrm{Tr}\Big(\check{\varrho}_0(\lambda,0)\sqrt{Y_1(\lambda,0)}J_{1,n}(\lambda-i0,0)\sqrt{Y_1(\lambda,0)}\check{Q}(\lambda,0)\\ \times\sqrt{Y_1(\lambda,0)}J_{1,n}(\lambda+i0,0)\sqrt{Y_1(\lambda,0)}\Big).\end{aligned}\tag{5.24}$$

Proposition 5.2.9 gives us

$$\begin{aligned}\lim_{\delta\to+0}\lim_{\epsilon\to+0}\mathrm{Tr}\Big(\Im\mathrm{m}\Big[\big(\Phi_{K_0}\varrho_0W_{1,-}^*(\epsilon)V_1Q_n\widetilde{W}_{1,-}(\epsilon)\Phi_{K_0}^*\big)(\lambda)\Big]\Big)\\ =\pi\int_{\Lambda_n^\varphi}\mathrm{d}\lambda\,\chi_{\Lambda_n^\varphi(0)}(\lambda)\mathrm{Tr}\big(\check{\varrho}_0(\lambda,0)\check{T}_1^*(\lambda,0)\check{Q}(\lambda,0)\check{T}_1(\lambda,0)\big).\end{aligned}$$

Note that $T_1(0)$ is trace class, whence $\int_{\mathbb{R}}\mathrm{d}\lambda\|\check{T}(\lambda,0)\|_1<\infty$. It follows that we can combine (5.24) with (5.23) and take the limit $n\to\infty$ to finally get

$$\lim_{n\to+\infty}\mathrm{Tr}\big(\varrho_0\Sigma_1(n)\big)=\int_{\mathbb{R}}\mathrm{d}\lambda\,\mathrm{Tr}\Big(\Im\mathrm{m}[\check{\varrho}_0(\lambda)\check{T}_1^*(\lambda)\check{Q}(\lambda)]-\pi\check{\varrho}_0(\lambda)\check{T}_1^*(\lambda)\check{Q}(\lambda)\check{T}_1(\lambda)\big)\Big).$$

□

We have calculated the first summand Σ_1 in the decomposition

$$\mathfrak{J}_Q=\lim_{n\to\infty}\lim_{\epsilon\to+0}\lim_{\delta\to+0}-2\,\Im\mathrm{m}\big[\mathrm{Tr}\big(\varrho_0(\Sigma_1(n)+\Sigma_2(\epsilon,\delta,n)+\Sigma_3(\epsilon,\delta,n)+\Sigma_4(\epsilon,\delta,n))\big)\big].$$

The calculation of Σ_2 is easy since it is similar to the trace class case of Chapter 3.

Lemma 5.2.11. *We have*

$$\begin{aligned}\lim_{n\to\infty}\lim_{\epsilon\to+0}\lim_{\delta\to+0}\Im\mathrm{m}\big[\mathrm{Tr}\big(\varrho_0\Sigma_2(\epsilon,\delta,n)\big)\big]\\ =\int_{\mathbb{R}}\mathrm{d}\lambda\,\Im\mathrm{m}\big[\mathrm{Tr}\big(\check{\varrho}_0(\lambda)\check{W}_{1,-}^*(\lambda)\check{T}_2^*(\lambda)\check{W}_{1,+}(\lambda)\check{Q}(\lambda)\big)\big].\end{aligned}\tag{5.25}$$

Proof. Recall $\Sigma_2(\epsilon,\delta,n)=W_{1,-}^*(n)\big(W_{2,-}^*(\epsilon,n)V_2W_{1,+}(\delta,n)+F^*(\epsilon,\delta,n)\big)Q_n$. First we show that $F^*(\epsilon,\delta,n)$ does not give any contribution since the trace vanishes in the limit. Note that, using Lemma 5.2.7,

$$\begin{aligned}&\big(\Phi_{K_1}F^*(\epsilon,\delta,n)g\big)(\lambda)\\ &=\Big(\Phi_{K_1}\int_{\mathbb{R}}\mathrm{d}E_{K_1}(\eta)P_1(\Lambda_n)C_2J_{2,n}(\eta-i\epsilon)C_2\int_{\mathbb{R}}(K_{1,n}-\nu+i\delta)^{-1}V_1P_0(\Lambda_n)\mathrm{d}E_0^{ac}(\nu)\\ &\quad-\int_{\mathbb{R}}\mathrm{d}E_{K_1}(\eta)P_1(\Lambda_n)C_2J_{2,n}(\eta-i\epsilon)C_2(K_{1,n}-\eta+i\epsilon)^{-1}\int_{\mathbb{R}}V_1P_{0,n}^{ac}\mathrm{d}E_0^{ac}(\nu)g\Big)(\lambda)\\ &=\mathcal{M}\big(\chi_{\Lambda_n^\varphi(\mu)}(\lambda)\big)\sqrt{Y_2(\lambda)}J_{2,n}(\lambda-i\epsilon)C_2\int_{\mathbb{R}}\mathrm{d}\nu\,(K_{1,n}-\nu+i\delta)^{-1}C_1^*Z_1\sqrt{Y_1(\nu)}\check{g}(\nu)\\ &\quad-\mathcal{M}\big(\chi_{\Lambda_n^\varphi(\mu)}(\lambda)\big)\sqrt{Y_2(\lambda)}J_{2,n}(\lambda-i\epsilon)C_2(K_{1,n}-\lambda+i\epsilon)^{-1}\int_{\mathbb{R}}\mathrm{d}\nu\,C_1^*Z_1\sqrt{Y_1(\nu)}\check{g}(\nu).\end{aligned}\tag{5.26}$$

Hence,

$$\begin{aligned}
&\operatorname{Tr}\big(\varrho_0 W_{1,-}^*(n) F^*(\epsilon,\delta,n) Q_n\big) \\
&\quad = \int_{\Lambda_n^\varphi(0)} \mathrm{d}\lambda \operatorname{Tr}\Big(\check{\varrho}_0(\lambda)\check{W}_{1,-}^*(\lambda)\sqrt{Y_2(\lambda)}J_{2,n}(\lambda - i\epsilon)C_2 \\
&\qquad\qquad \times \big((K_{1,n} - \lambda + i\delta)^{-1} - (K_{1,n} - \lambda + i\epsilon)^{-1}\big) C_1^* Z_1 \sqrt{Y_1(\lambda)}\check{Q}(\lambda)\Big)
\end{aligned}$$

Since $C_2(K_{1,n} - \lambda + i\delta)^{-1}C_1^*$ and $C_2(K_{1,n} - \lambda + i\delta)^{-1}C_1^*$ converge uniformly in $\lambda \in \Lambda_n^\varphi$ in the Hilbert-Schmidt norm as $\delta \to +0$, it follows that

$$\lim_{\epsilon\to+0}\lim_{\delta\to+0} \operatorname{Tr}\big(\varrho_0 W_{1,-}^*(n) F^*(\epsilon,\delta,n) Q_n\big) = 0.$$

We are left with

$$\begin{aligned}
&\lim_{\epsilon\to+0}\lim_{\delta\to+0} \operatorname{Tr}(\varrho_0 \Sigma_2(\epsilon,n)) \\
&\quad = \lim_{\epsilon\to+0}\lim_{\delta\to+0} \operatorname{Tr}\big(\varrho_0 W_{1,-}^*(n) W_{2,-}^*(\epsilon,n) V_2 W_{1,+}(\delta,n) Q_n\big) \\
&\quad = \lim_{\epsilon\to+0} \int_{\Lambda_n^\varphi(0)} \mathrm{d}\lambda \operatorname{Tr}\Big(\check{\varrho}_0(\lambda)\check{W}_{1,-}^*(\lambda)(\Phi_{K_1} W_{2,-}^*(\epsilon,n) V_2 P_1(\Lambda_n)\Phi_{K_1}^*)(\lambda,\lambda)\check{W}_{1,+}(\lambda)\check{Q}_n(\lambda)\Big)
\end{aligned} \tag{5.27}$$

We conclude the proof by calculating $\check{T}_2^*(\lambda) = (\Phi_{K_1} W_{2,-}^* V_2 \Phi_{K_1}^*)(\lambda,\lambda)$ analogously to the proof of Lemma 5.2.10. We have $W_{2,-}^* V_2 = \lim_{\epsilon\to+0} W_{2,-}^*(\epsilon) V_2$ in trace norm and

$$\begin{aligned}
&(\Phi_{K_1} W_{2,-}^*(\epsilon,n) V_2 P_1(\Lambda_n)\Phi_{K_1}^* f)(\lambda) \\
&\quad = (\Phi_{K_1} \int_{\mathbb{R}} P_1(\Lambda_n)\mathrm{d}E_{K_1}(\nu) C_2 J_{2,n}(\nu - i\epsilon) C_2 \int_{\mathbb{R}} \mathrm{d}E_{K_1}(\eta) P_1(\Lambda_n) f)(\lambda) \\
&\quad = \mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\sqrt{Y_2(\lambda)}J_{2,n}(\lambda - i\epsilon) \int_{\mathbb{R}} \mathrm{d}\eta \sqrt{Y_2(\eta)}\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\eta))\check{f}(\eta)
\end{aligned}$$

Taking the diagonal of the kernel and the limit $\epsilon \to +0$, we obtain

$$\begin{aligned}
&(\Phi_{K_1} W_{2,-}^* V_2 P_1(\Lambda_n)\Phi_{K_1}^*)(\lambda,\lambda) \\
&\quad = \mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\sqrt{Y_2(\lambda)}J_{2,n}(\lambda - i0)\sqrt{Y_2(\lambda)}\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda)) \\
&\quad = \mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\check{T}_2^*(\lambda)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))
\end{aligned}$$

from (5.12). We insert this into (5.27) and use $P_1(\Lambda_n)W_{1,\pm}(n) = W_{1,\pm}(n)P_{0,n}^{ac}$ to obtain

$$\begin{aligned}
&\lim_{n\to\infty}\lim_{\epsilon\to+0}\lim_{\delta\to+0} \operatorname{Tr}\big(\varrho_0 \Sigma_2(\epsilon,\delta,n)\big) \\
&\quad = \lim_{n\to\infty} \int_{\mathbb{R}} \mathrm{d}\lambda \operatorname{Tr}\big(\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\check{\varrho}_0(\lambda)\check{W}_{1,-}^*(\lambda)\check{T}_2^*(\lambda)\check{W}_{1,+}(\lambda)\check{Q}(\lambda)\big) \\
&\quad = \lim_{n\to\infty} \int_{\Lambda_n^\varphi(0)} \mathrm{d}\lambda \operatorname{Tr}\big(\check{\varrho}_0(\lambda,0)\check{W}_{1,-}^*(\lambda,0)\check{T}_2^*(\lambda)(0,0)\check{W}_{1,+}(\lambda,0)\check{Q}(\lambda,0)\big) \\
&\quad = \int_{\mathbb{R}} \mathrm{d}\lambda \operatorname{Tr}\big(\check{\varrho}_0(\lambda)\check{W}_{1,-}^*(\lambda)\check{T}_2^*(\lambda)\check{W}_{1,+}(\lambda)\check{Q}(\lambda)\big).
\end{aligned} \tag{5.28}$$

□

It remains to calculate the contributions of $\Sigma_3(\epsilon,\delta,n)$ and $\Sigma_4(\epsilon,\delta,n)$ in (5.18). The calculations of the contributions of $\Sigma_3(\epsilon,\delta,n)$ and $\Sigma_4(\epsilon,\delta,n)$ are more involved than those of Σ_1 and Σ_2, but they are similar in many respects. However, the case of $\Sigma_4(\epsilon,\delta,n)$ is slightly less complicated, whence we start with the calculation of this term. Let us first prove two lemmas that will be of use for this. They use the spectral representation $\Phi_{2,0}$ of K_0^{ac} that we obtain from

$$Y_{2,0}(\lambda) = \frac{\mathrm{d}}{\mathrm{d}\lambda} C_2 E_{K_0}(\lambda) C_2$$

and Lemma 3.1.4. Let

$$\begin{aligned}\mathcal{G}(\lambda,\epsilon,n) = C_2(1-(K_{1,n}-\lambda+i\epsilon)^{-1}V_1)\int_{\mathbb{R}} \mathrm{d}E_0^{ac}(\xi)Q_n \\ \times \int_{\mathbb{R}} \mathrm{d}E_0^{ac}(\gamma)(\gamma-\lambda-i\epsilon)^{-1}(1-V_1(K_{1,n}-\lambda-i\epsilon)^{-1})C_2\end{aligned}$$

The following lemma gives us a representation of $\mathcal{G}$ using $\Phi_{2,0}$ and proves that the limits exist for $\epsilon \to +0$.

Lemma 5.2.12. *For every $n \in \mathbb{N}$ and a.e. $\lambda \in \Lambda_n^{\varphi}$, we have*

$$\mathcal{G}(\lambda,\epsilon,n) = \int_{\mathbb{R}} \mathrm{d}\xi\; G_{\epsilon,n}^*(\lambda,\xi)\check{Q}(\xi)\mathcal{M}(\chi_{\Lambda_n^{\varphi}(\mu)}(\xi))G_{\epsilon,n}(\lambda,\xi)(\gamma-\lambda-i\epsilon)^{-1}. \tag{5.29}$$

Here,

$$G_{\epsilon,n}(\lambda,\xi) = (\Phi_{K_0}\Phi_{2,0}^*)(\xi)\sqrt{Y_{2,0}(\xi)} - \sqrt{Y_1(\xi)}Z_1C_1(K_{1,n}-\lambda-i\epsilon)^{-1}C_2 \tag{5.30}$$

and the limit $G_{0,n}(\lambda,\xi) = \lim_{\epsilon\to+0} G_{\epsilon,n}(\lambda,\xi)$ exists in the Hilbert-Schmidt norm for a.e. $\lambda,\xi \in \Lambda_n^{\varphi}$ and every $n \in \mathbb{N}$. Furthermore, it converges uniformly in λ for $\lambda \in \Lambda_n^{\varphi}$.

Proof. First note that Lemma 3.1.5 holds for $\Phi_{2,0}$. We have

$$\begin{aligned}\mathcal{G}(\lambda,\epsilon) = \int_{\mathbb{R}} C_2\mathrm{d}E_0^{ac}(\xi)\Phi_{2,0}^*\Phi_{2,0}Q_n\Phi_{2,0}^*\Phi_{2,0}\int_{\mathbb{R}}\mathrm{d}E_0^{ac}(\nu)C_2(\nu-\lambda-i\epsilon)^{-1} \\ - C_2(K_{1,n}-\lambda+i\epsilon)^{-1}\int_{\mathbb{R}} V_1\mathrm{d}E_0^{ac}(\xi)\Phi_{K_0}^*\Phi_{K_0}Q_n\Phi_{2,0}^* \\ \times \Phi_{2,0}\int_{\mathbb{R}}\mathrm{d}E_0^{ac}(\nu)C_2(\nu-\lambda-i\epsilon)^{-1} \\ - \int_{\mathbb{R}} C_2\mathrm{d}E_0^{ac}(\xi)\Phi_{2,0}^*\Phi_{2,0}Q_n\Phi_{K_0}^*\Phi_{K_0}\int_{\mathbb{R}}\mathrm{d}E_0^{ac}(\nu)C_1^* \\ \times (\nu-\lambda-i\epsilon)^{-1}Z_1C_1(K_{1,n}-\lambda-i\epsilon)^{-1}C_2 \\ + (K_{1,n}-\lambda+i\epsilon)^{-1}\int_{\mathbb{R}} V_1\mathrm{d}E_0^{ac}(\xi)\Phi_{K_0}^*\Phi_{K_0}Q_n\Phi_{K_0}^*\Phi_{K_0}\int_{\mathbb{R}}\mathrm{d}E_0^{ac}(\nu)C_1^* \\ \times (\nu-\lambda-i\epsilon)^{-1}Z_1C_1(K_{1,n}-\lambda-i\epsilon)^{-1}C_2,\end{aligned}$$

whence

$$\begin{aligned}\mathcal{G}(\lambda,\epsilon) = \int_{\mathbb{R}} \mathrm{d}\xi\, \sqrt{Y_{2,0}(\xi)}(\Phi_{2,0}\Phi_{K_0}^*)(\xi)\check{Q}(\xi)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\xi))(\Phi_{K_0}\Phi_{2,0}^*)(\xi) \\ \times \sqrt{Y_{2,0}(\xi)}(\xi-\lambda-i\epsilon)^{-1} \\ - \int_{\mathbb{R}} \mathrm{d}\xi\, C_2(K_{1,n}-\lambda+i\epsilon)^{-1}C_1^* Z_1\sqrt{Y_1(\xi)}\check{Q}(\xi)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\xi)) \\ \times (\Phi_{K_0}\Phi_{2,0}^*)(\xi)\sqrt{Y_{2,0}(\xi)}(\xi-\lambda-i\epsilon)^{-1} \\ - \int_{\mathbb{R}} \mathrm{d}\xi\, \sqrt{Y_{2,0}(\xi)}(\Phi_{2,0}\Phi_{K_0}^*)(\xi)\check{Q}(\xi)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\xi))(\xi-\lambda-i\epsilon)^{-1} \\ \times \sqrt{Y_1(\xi)}Z_1C_1(K_{1,n}-\lambda-i\epsilon)^{-1}C_2 \\ + \int_{\mathbb{R}} \mathrm{d}\xi\, C_2(K_{1,n}-\lambda+i\epsilon)^{-1}C_1^* Z_1\sqrt{Y_1(\xi)}\check{Q}(\xi)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\xi))(\xi-\lambda-i\epsilon)^{-1} \\ \times \sqrt{Y_1(\xi)}Z_1C_1(K_{1,n}-\lambda-i\epsilon)^{-1}C_2.\end{aligned}$$

Summing up the terms results in the first statement of the lemma, relation (5.29). The limit $G_\epsilon(\lambda,\xi) \xrightarrow{\epsilon\to+0} G_0(\lambda,\xi)$ exists in the Hilbert-Schmidt norm by Proposition 5.2.2 since C_1 is $K_{1,n}$-smooth by Proposition 5.2.3 and C_2 is Hilbert-Schmidt by Proposition 5.3.1. By construction of Λ_n, the convergence of $C_1(K_1-\lambda-i\epsilon)^{-1}C_2$ as $\epsilon\to+0$ is uniform in λ for $\lambda\in\Lambda_n$. □

Lemma 5.2.13. *We have*

$$\begin{aligned}&G_{0,n}^*(\lambda,\lambda)\check{Q}(\lambda)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))G_{0,n}(\lambda,\lambda) \\ &\quad= \lim_{\epsilon\to+0} G_{\epsilon,n}^*(\lambda,\lambda)\check{Q}(\lambda)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))G_{\epsilon,n}(\lambda,\lambda) \\ &\quad= \sqrt{Y_2(\lambda)}\check{W}_{1,+}(\lambda)\check{Q}(\lambda)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\check{W}_{1,+}^*(\lambda)\sqrt{Y_2(\lambda)}\end{aligned} \tag{5.31}$$

for a.e. $\lambda\in\Lambda_n$, $n\in\mathbb{N}$, where the limit is taken in the Hilbert-Schmidt norm.

Proof. Let $n\in\mathbb{N}$ and $\lambda\in\Lambda_n$. We know that

$$\begin{aligned}&\sqrt{Y_2(\lambda)}\check{W}_{1,+}(\lambda)\check{Q}(\lambda)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\check{W}_{1,+}^*(\lambda)\sqrt{Y_2(\lambda)} \\ &\quad= \lim_{\epsilon\to+0}\int_{\mathbb{R}} \mathrm{d}\nu\, \pi^{-1}\tfrac{\epsilon}{(\lambda-\nu)^2+\epsilon^2}\sqrt{Y_2(\nu)}\check{W}_{1,+}(\nu)\check{Q}(\nu)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\nu))\check{W}_{1,+}^*(\nu)\sqrt{Y_2(\nu)}.\end{aligned}$$

Using Lemma 3.1.5 and the intertwining property of the wave operator gives us

$$\begin{aligned}&\sqrt{Y_2(\lambda)}\check{W}_{1,+}(\lambda)\check{Q}(\lambda)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\xi))\check{W}_{1,+}^*(\lambda)\sqrt{Y_2(\lambda)} \\ &\quad= \lim_{\epsilon\to+0} C_2\int_{\mathbb{R}} \pi^{-1}\tfrac{\epsilon}{(\lambda-\nu)^2+\epsilon^2}\mathrm{d}E_{K_1}(\nu)W_{1,+}(n)Q_nW_{1,+}^*(n)\int_{\mathbb{R}}\mathrm{d}E_{K_1}(\eta)C_2 \\ &\quad= \lim_{\epsilon\to+0} C_2W_{1,+}(n)\int_{\mathbb{R}} \pi^{-1}\tfrac{\epsilon}{(\lambda-\nu)^2+\epsilon^2}\mathrm{d}E_0^{ac}(\nu)Q_n\int_{\mathbb{R}}\mathrm{d}E_0^{ac}(\eta)W_{1,+}^*(n)C_2.\end{aligned}$$

Since $C_2 W_{1,+}(\epsilon, n) \xrightarrow{\epsilon \to +0} C_2 W_{1,+}(n)$ in the Hilbert-Schmidt norm,

$$\begin{aligned}
&\sqrt{Y_2(\lambda)}\check{W}_{1,+}(\lambda)\check{Q}(\lambda)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\check{W}_{1,+}^*(\lambda)\sqrt{Y_2(\lambda)} \\
&\quad = \lim_{\epsilon\to+0}\lim_{\delta\to+0}\lim_{\varepsilon\to+0}\int_{\mathbb{R}} \pi^{-1}\tfrac{\epsilon}{(\lambda-\nu)^2+\epsilon^2}(C_2 - C_2(K_{1,n}-\nu+i\delta)^{-1}V_1)\mathrm{d}E_0^{ac}(\nu)Q_n \\
&\qquad\qquad \times \int_{\mathbb{R}} \mathrm{d}E_0^{ac}(\eta)(C_2 - V_1(K_{1,n}-\eta-i\varepsilon)^{-1}C_2).
\end{aligned}$$

We proceed as in the proof of Lemma 5.2.12. Namely,

$$\begin{aligned}
&\int_{\mathbb{R}} \pi^{-1}\tfrac{\epsilon}{(\lambda-\nu)^2+\epsilon^2}(C_2 - C_2(K_{1,n}-\nu+i\delta)^{-1}V_1)\mathrm{d}E_0^{ac}(\nu)Q_n \\
&\qquad\qquad \times \int_{\mathbb{R}} \mathrm{d}E_0^{ac}(\eta)(C_2 - V_1(K_{1,n}-\eta-i\varepsilon)^{-1}C_2) \\
&\quad = \int_{\mathbb{R}} \mathrm{d}\nu\, \pi^{-1}\tfrac{\epsilon}{(\lambda-\nu)^2+\epsilon^2}\sqrt{Y_{2,0}(\nu)}(\Phi_{2,0}\Phi_{K_0}^*)(\nu)\check{Q}(\nu)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\nu)) \\
&\qquad\qquad \times (\Phi_{K_0}\Phi_{2,0}^*)(\nu)\sqrt{Y_{2,0}(\nu)} \\
&\qquad - \int_{\mathbb{R}} \mathrm{d}\nu\, \pi^{-1}\tfrac{\epsilon}{(\lambda-\nu)^2+\epsilon^2}C_2(K_{1,n}-\nu+i\delta)^{-1}C_1^*Z_1 \\
&\qquad\qquad \times \sqrt{Y_1(\nu)}\check{Q}(\nu)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\nu))(\Phi_{K_0}\Phi_{2,0}^*)(\nu)\sqrt{Y_{2,0}(\nu)} \\
&\qquad - \int_{\mathbb{R}} \mathrm{d}\nu\, \pi^{-1}\tfrac{\epsilon}{(\lambda-\nu)^2+\epsilon^2}\sqrt{Y_{2,0}(\nu)}(\Phi_{2,0}\Phi_{K_0}^*)(\nu)\check{Q}(\nu)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\nu)) \\
&\qquad\qquad \times \sqrt{Y_1(\nu)}Z_1C_1(K_{1,n}-\nu-i\varepsilon)^{-1}C_2 \\
&\qquad + \int_{\mathbb{R}} \mathrm{d}\nu\, \pi^{-1}\tfrac{\epsilon}{(\lambda-\nu)^2+\epsilon^2}C_2(K_{1,n}-\nu+i\delta)^{-1}C_1^*Z_1\sqrt{Y_1(\nu)}\check{Q}(\nu) \\
&\qquad\qquad \times \mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\nu))\sqrt{Y_1(\nu)}Z_1C_1(K_{1,n}-\nu-i\varepsilon)^{-1}C_2.
\end{aligned} \tag{5.32}$$

By Lemma 5.2.12 the limit of $C_1(K_{1,n}-\nu-i\epsilon)^{-1}C_2$ as $\epsilon \to +0$ exists in the Hilbert-Schmidt norm. It converges uniformly on Λ_n^φ by construction of Λ_n^φ. Hence, we can take the limit in (5.32) and obtain, after summing up the terms and taking into account the definition (5.30) of G_0,

$$\begin{aligned}
&\sqrt{Y_2(\lambda)}\check{W}_{1,+}(\lambda)\check{Q}(\lambda)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\check{W}_{1,+}^*(\lambda)\sqrt{Y_2(\lambda)} \\
&\quad = \sqrt{Y_{2,0}(\lambda)}(\Phi_{2,0}\Phi_{K_0}^*)(\lambda)\check{Q}(\lambda)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))(\Phi_{K_0}\Phi_{2,0}^*)(\lambda)\sqrt{Y_{2,0}(\lambda)} \\
&\qquad - C_2(K_{1,n}-\lambda+i0)^{-1}C_1^*Z_1\sqrt{Y_1(\lambda)}\check{Q}(\lambda)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))(\Phi_{K_0}\Phi_{2,0}^*)(\lambda)\sqrt{Y_{2,0}(\lambda)} \\
&\qquad - \sqrt{Y_{2,0}(\lambda)}(\Phi_{2,0}\Phi_{K_0}^*)(\lambda)\check{Q}(\lambda)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\sqrt{Y_1(\lambda)}Z_1C_1(K_{1,n}-\lambda-i0)^{-1}C_2 \\
&\qquad + C_2(K_{1,n}-\lambda+i0)^{-1}C_1^*Z_1\sqrt{Y_1(\lambda)}\check{Q}(\lambda)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\sqrt{Y_1(\lambda)} \\
&\qquad\qquad \times Z_1C_1(K_{1,n}-\lambda-i0)^{-1}C_2 \\
&\quad = G_{0,n}^*(\lambda,\lambda)\check{Q}(\lambda)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))G_{0,n}(\lambda,\lambda).
\end{aligned}$$

□

Lemma 5.2.14. *We have*

$$\begin{aligned}&\lim_{n\to\infty}\lim_{\epsilon\to+0}\lim_{\delta\to+0}\Im\mathrm{m}\big[\mathrm{Tr}\big(\varrho_0\Sigma_4(\epsilon,\delta,n)\big)\big]\\&\qquad=\pi\int_{\mathbb{R}}\mathrm{d}\lambda\,\mathrm{Tr}\Big(\check{\varrho}_0(\lambda)\check{W}^*_{1,-}(\lambda)\check{T}^*_2(\lambda)\check{W}_{1,+}(\lambda)\check{Q}(\lambda)\check{W}_{1,+}(\lambda)\check{T}_2(\lambda)\check{W}_{1,-}(\lambda)\Big)\end{aligned}\tag{5.33}$$

Proof. Recall that

$$\Sigma_4(\epsilon,\delta,n)=-W^*_{1,-}(n)\big(W^*_{2,-}(\epsilon,n)V_2W_{1,+}(\delta,n)+F^*(\epsilon,\delta,n)\big)Q_n\widetilde{W}_{2,-}(\epsilon,n)W_{1,-}(n).$$

Using (5.17) gives us

$$\begin{aligned}&W^*_{2,-}(\epsilon,n)V_2W_{1,+}(\delta,n)+F^*(\epsilon,\delta,n)\\&=\int_{\mathbb{R}}\mathrm{d}E_{K_1}(\gamma)P_1(\Lambda_n)C_2J_{2,n}(\gamma-i\epsilon)C_2\int_{\mathbb{R}}\big(1-(K_{1,n}-\nu+i\delta)^{-1}V_1\big)P_0(\Lambda_n)\mathrm{d}E^{ac}_0(\nu)\\&\quad+\int_{\mathbb{R}}\mathrm{d}E_{K_1}(\gamma)P_1(\Lambda_n)C_2J_{2,n}(\gamma-i\epsilon)C_2\int_{\mathbb{R}}(K_{1,n}-\nu+i\delta)^{-1}V_1P_0(\Lambda_n)\mathrm{d}E^{ac}_0(\nu)\\&\quad-\int_{\mathbb{R}}\mathrm{d}E_{K_1}(\gamma)P_1(\Lambda_n)C_2J_{2,n}(\gamma-i\epsilon)C_2(K_{1,n}-\gamma+i\epsilon)^{-1}\int_{\mathbb{R}}V_1P_0(\Lambda_n)\mathrm{d}E^{ac}_0(\nu)\\&=\int_{\mathbb{R}}\mathrm{d}E_{K_1}(\gamma)P_1(\Lambda_n)C_2J_{2,n}(\gamma-i\epsilon)C_2(1-(K_{1,n}-\gamma+i\epsilon)^{-1}V_1)\int_{\mathbb{R}}P_0(\Lambda_n)\mathrm{d}E^{ac}_0(\nu).\end{aligned}\tag{5.34}$$

Furthermore,

$$\begin{aligned}&P^{ac}_{0,n}\widetilde{W}_{2,-}(\epsilon,n)\\&=P^{ac}_{0,n}\int_{\mathbb{R}}(K_{2,n}-\eta-i\epsilon)^{-1}V_2P_1(\Lambda_n)\mathrm{d}E_{K_1}(\eta)\\&=\int_{\mathbb{R}}\mathrm{d}E^{ac}_0(\gamma)P_0(\Lambda_n)\int_{\mathbb{R}}(K_{1,n}-\eta-i\epsilon)^{-1}C_2J_{2,n}(\eta+i\epsilon)C_2P_1(\Lambda_n)\mathrm{d}E_{K_1}(\eta)\\&=\int_{\mathbb{R}}\mathrm{d}E^{ac}_0(\gamma)P_0(\Lambda_n)\int_{\mathbb{R}}(K_{0,n}-\eta-i\epsilon)^{-1}(1-V_1(K_{1,n}-\eta-i\epsilon)^{-1})\\&\qquad\qquad\times C_2J_{2,n}(\eta+i\epsilon)C_2P_1(\Lambda_n)\mathrm{d}E_{K_1}(\eta).\end{aligned}\tag{5.35}$$

Passing to the spectral representation and using Lemma 3.1.5, we obtain

$$\begin{aligned}&\Big(\Phi_{K_0}W^*_{1,-}(n)\big(W^*_{2,-}(\epsilon,n)V_2W_{1,+}(\delta,n)+F(\epsilon,\delta,n)^*\big)\\&\qquad\qquad\times Q_n\widetilde{W}_{2,-}(\epsilon,n)W_{1,-}(n)\Phi^*_{K_0}\check{f}\Big)(\lambda)\\&=\mathcal{M}(\chi_{\Lambda^\varphi_n(\mu)}(\lambda))\check{W}^*_{1,-}(\lambda)\Big(\Phi_{K_1}\int_{\mathbb{R}}\mathrm{d}E_{K_1}(\nu)P_1(\Lambda_n)C_2J_{2,n}(\nu-i\epsilon)C_2\\&\qquad\times(1-(K_{1,n}-\nu+i\epsilon)^{-1}V_1)\int_{\mathbb{R}}P_0(\Lambda_n)\mathrm{d}E^{ac}_0(\xi)Q_n\int_{\mathbb{R}}\mathrm{d}E^{ac}_0(\gamma)\\&\qquad\times\int_{\mathbb{R}}(K_{0,n}-\eta-i\epsilon)^{-1}(1-V_1(K_{1,n}-\eta-i\epsilon)^{-1})C_2J_{2,n}(\eta+i\epsilon)\\&\qquad\qquad\times C_2P_1(\Lambda_n)\mathrm{d}E_{K_1}(\eta)\Phi^*_{K_1}\Phi_{K_1}W_{1,-}(n)\Phi^*_{K_0}\check{f}\Big)(\lambda).\end{aligned}$$

Thus,

$$\begin{aligned}
&\Big(\Phi_{K_0} W_{1,-}^*(n)\big(W_{2,-}^*(\epsilon,n)V_2 W_{1,+}(\delta,n) + F(\epsilon,\delta,n)^*\big) \\
&\qquad\qquad \times Q_n \widetilde{W}_{2,-}(\epsilon,n) W_{1,-}(n)\Phi_{K_0}^* \check{f}\Big)(\lambda) \\
&= \mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\check{W}_{1,-}^*(\lambda)\sqrt{Y_2(\lambda)}J_{2,n}(\lambda - i\epsilon)C_2\big(1-(K_{1,n}-\lambda+i\epsilon)^{-1}V_1\big) \\
&\quad \times \int_{\mathbb{R}} P_0(\Lambda_n)\mathrm{d}E_0^{ac}(\xi)Q_n \int_{\mathbb{R}}\mathrm{d}\eta \int_{\mathbb{R}}\mathrm{d}E_0^{ac}(\gamma)(\gamma-\eta-i\epsilon)^{-1} \\
&\quad \times \big(1-V_1(K_{1,n}-\eta-i\epsilon)^{-1}\big)C_2 J_{2,n}(\eta+i\epsilon)\sqrt{Y_2(\eta)} \\
&\qquad\qquad \times \check{W}_{1,-}(\eta)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\eta))\check{f}(\eta)
\end{aligned}$$

for $\check{f} \in L^2\big(\mathbb{R}, \mathrm{d}\lambda, \mathfrak{H}_\lambda\big)$, which gives us

$$\begin{aligned}
&\Big(\Phi_{K_0} W_{1,-}^*(n)\big(W_{2,-}^*(\epsilon,n)V_2 W_{1,+}(\delta,n) + F(\epsilon,\delta,n)^*\big) \\
&\qquad\qquad \times Q_n \widetilde{W}_{2,-}(\epsilon,n) W_{1,-}(n)\Phi_{K_0}^* \check{f}\Big)(\lambda) \\
&= \mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\check{W}_{1,-}^*(\lambda)\sqrt{Y_2(\lambda)}J_{2,n}(\lambda - i\epsilon)C_2\big(1-(K_{1,n}-\lambda+i\epsilon)^{-1}V_1\big) \\
&\quad \times \int_{\mathbb{R}} P_0(\Lambda_n)\mathrm{d}E_0^{ac}(\xi)Q_n \int_{\mathbb{R}}\mathrm{d}\eta \int_{\mathbb{R}}\mathrm{d}E_0^{ac}(\gamma)(\gamma-\eta-i\epsilon)^{-1} \\
&\quad \times \big(1-V_1(K_{1,n}-\eta-i\epsilon)^{-1}\big)C_2 J_{2,n}(\eta+i\epsilon)\sqrt{Y_2(\eta)} \\
&\qquad\qquad \times \check{W}_{1,-}(\eta)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\eta))\check{f}(\eta).
\end{aligned}$$

We include the multiplication operator ϱ_0 and obtain an integral operator for which we can calculate the trace as

$$\begin{aligned}
&\Im\mathrm{m}\Big[\mathrm{Tr}\Big(\varrho_0 W_{1,-}^*(n)\big(W_{2,-}^*(\epsilon,n)V_2 W_{1,+}(\delta,n) + F^*(\epsilon,\delta,n)\big)Q_n\widetilde{W}_{2,-}(\epsilon,n)W_{1,-}(n)\Big)\Big] \\
&= \int_{\mathbb{R}}\mathrm{d}\lambda\,\Im\mathrm{m}\Big[\mathrm{Tr}\Big(\check{\varrho}_0(\lambda)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\check{W}_{1,-}^*(\lambda)\sqrt{Y_2(\lambda)}J_{2,n}(\lambda-i\epsilon)C_2 \\
&\qquad\qquad \times \big(1-(K_{1,n}-\lambda+i\epsilon)^{-1}V_1\big)\int_{\mathbb{R}}\mathrm{d}E_0^{ac}(\xi)Q_n\int_{\mathbb{R}}\mathrm{d}E_0^{ac}(\gamma) \\
&\qquad\qquad \times (\gamma-\lambda-i\epsilon)^{-1}\big(1-V_1(K_{1,n}-\lambda-i\epsilon)^{-1}\big)C_2J_{2,n}(\lambda+i\epsilon) \\
&\qquad\qquad\qquad \times \sqrt{Y_2(\lambda)}\check{W}_{1,-}(\lambda)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\Big)\Big] \\
&= \int_{\mathbb{R}}\mathrm{d}\lambda\,\mathrm{Tr}\Big(\check{\varrho}_0(\lambda)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\check{W}_{1,-}^*(\lambda)\sqrt{Y_2(\lambda)}J_{2,n}(\lambda-i\epsilon)\int_{\mathbb{R}}\mathrm{d}\xi G_{\epsilon,n}^*(\lambda,\xi)\check{Q}(\xi) \\
&\qquad\qquad \times \mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\xi))G_{\epsilon,n}(\lambda,\xi)\tfrac{\epsilon}{(\xi-\lambda)^2+\epsilon^2}J_{2,n}(\lambda+i\epsilon)\sqrt{Y_2(\lambda)}\check{W}_{1,-}(\lambda)\Big),
\end{aligned}$$

where we used Lemma 5.2.12. Since $G_\epsilon(\lambda,\xi)$ converges uniformly in λ for $\lambda \in \Lambda_n^\varphi$ and decomposes into summands that factorize with respect to ξ and λ, where the ξ-dependent

factor is independent of ϵ, we can take the limit and get

$$\begin{aligned}
&\lim_{\epsilon\to+0} \Im\mathrm{m}\Big[\mathrm{Tr}\Big(\varrho_0 W_{1,-}^*(n)\big(W_{2,-}^*(\epsilon,n)V_2W_{1,+}(\delta,n)+F^*(\epsilon,\delta,n)\big)\\
&\qquad\qquad\qquad\qquad\times Q_n\widetilde{W}_{2,-}(\epsilon,n)W_{1,-}(n)\Big)\Big]\\
&=\pi\int_{\mathbb{R}}\mathrm{d}\lambda\,\mathrm{Tr}\Big(\check{\varrho}_0(\lambda)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\check{W}_{1,-}^*(\lambda)\sqrt{Y_2(\lambda)}J_{2,n}(\lambda-i0)G_0^*(\lambda,\lambda)\\
&\qquad\qquad\times\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\check{Q}(\lambda)G_0(\lambda,\lambda)J_{2,n}(\lambda+i0)\sqrt{Y_2(\lambda)}\check{W}_{1,-}(\lambda)\Big).
\end{aligned}\tag{5.36}$$

We insert the relation (5.31) of Lemma 5.2.13 into (5.36) and use (5.12) to obtain

$$\begin{aligned}
&\lim_{\epsilon\to+0} -\Im\mathrm{m}\Big[\mathrm{Tr}\Big(\varrho_0 W_{1,-}^*(n)\big(W_{2,-}^*(\epsilon,n)V_2W_{1,+}(\delta,n)+F^*(\epsilon,\delta,n)\big)\\
&\qquad\qquad\qquad\qquad\times Q_n\widetilde{W}_{2,-}(\epsilon,n)W_{1,-}(n)\Big)\Big]\\
&=-\pi\int_{\mathbb{R}}\mathrm{d}\lambda\mathrm{Tr}\Big(\check{\varrho}_0(\lambda)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\check{W}_{1,-}^*(\lambda)\sqrt{Y_2(\lambda)}J_{2,n}(\lambda-i0)\sqrt{Y_2(\lambda)}\check{W}_{1,+}(\lambda)\\
&\qquad\qquad\times\check{Q}(\lambda)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\check{W}_{1,+}^*(\lambda)\sqrt{Y_2(\lambda)}J_{2,n}(\lambda+i0)\sqrt{Y_2(\lambda)}\check{W}_{1,-}(\lambda)\Big)\\
&=-\pi\int_{\Lambda_n(0)}\mathrm{d}\lambda\mathrm{Tr}\Big(\check{\varrho}_0(\lambda)\check{W}_{1,-}^*(\lambda)\check{T}_2^*(\lambda)\check{W}_{1,+}(\lambda)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\\
&\qquad\qquad\times\check{Q}(\lambda)\check{W}_{1,+}(\lambda)\check{T}_2(\lambda)\check{W}_{1,-}(\lambda)\Big).
\end{aligned}\tag{5.37}$$

Recall that T_2 is trace class and $\text{s-lim}_{n\to\infty}Q_n=Q$. Hence, $Q_nW_{1,+}T_2$ converges to $QW_{1,+}T_2$ in trace norm. In particular, this implies that

$$\lim_{n\to\infty}\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\check{Q}(\lambda)\check{W}_{1,+}(\lambda)\check{T}_2(\lambda)=\check{Q}(\lambda)\check{W}_{1,+}(\lambda)\check{T}_2(\lambda)$$

converges in the operator norm uniformly in λ. Thus, we can take the limit $n\to\infty$ in (5.37) and arrive at

$$\begin{aligned}
&\lim_{n\to\infty}\lim_{\epsilon\to+0} \Im\mathrm{m}\Big[\mathrm{Tr}\Big(\varrho_0 W_{1,-}^*(n)\big(W_{2,-}^*(\epsilon,n)V_2W_{1,+}(\delta,n)+F^*(\epsilon,\delta,n)\big)\\
&\qquad\qquad\qquad\qquad\times Q_n\widetilde{W}_{2,-}(\epsilon,n)W_{1,-}(n)\Big)\Big]\\
&=\pi\int_{\mathbb{R}}\mathrm{d}\lambda\,\mathrm{Tr}\Big(\check{\varrho}_0(\lambda)\check{W}_{1,-}^*(\lambda)\check{T}_2^*(\lambda)\check{W}_{1,+}(\lambda)\check{Q}(\lambda)\check{W}_{1,+}(\lambda)\check{T}_2(\lambda)\check{W}_{1,-}(\lambda)\Big).
\end{aligned}\tag{5.38}$$

□

Let us go back to equation (5.18). It remains to calculate the contribution of $\Sigma_3(\epsilon)$. The calculations are similar to those for $\Sigma_4(\epsilon)$. As before, we start with proving a simple lemma that is very much alike to Lemma 5.2.13, but adapted to the expression $\Sigma_3(\epsilon)$. From (5.30), recall the definition

$$G_{0,n}(\lambda,\xi)=\lim_{\epsilon\to+0}(\Phi_{K_0}\Phi_{2,0}^*)(\xi)\sqrt{Y_{2,0}(\xi)}-\sqrt{Y_1(\xi)}Z_1C_1(K_{1,n}-\lambda-i0)^{-1}C_2.$$

Lemma 5.2.15. *For a.e. $\lambda \in \Lambda_n$, we have*

$$\sqrt{Y_1(\lambda)}\check{Q}(\lambda)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))G_{0,n}(\lambda,\lambda) = \sqrt{Y_1(\lambda)}\check{Q}(\lambda)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\check{W}_{1,+}^*(\lambda)\sqrt{Y_2(\lambda)},$$

where the limit is taken in the Hilbert-Schmidt norm and the convergence is uniform in $\lambda \in \Lambda_n^\varphi$.

Proof. Just as in the proof of Lemma 5.2.13, we have

$$\begin{aligned}
&\sqrt{Y_1(\lambda)}\check{Q}(\lambda)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\check{W}_{1,+}^*(\lambda)\sqrt{Y_2(\lambda)} \\
&\quad = \lim_{\epsilon\to+0}\int_{\mathbb{R}} \pi^{-1}\tfrac{\epsilon}{(\lambda-\nu)^2+\epsilon^2}C_1\mathrm{d}E_0^{ac}(\nu)Q_nW_{1,+}^*(n)\int_{\mathbb{R}}\mathrm{d}E_{K_1}(\eta)C_2 \\
&\quad = \lim_{\epsilon\to+0}\lim_{\delta\to+0}\int_{\mathbb{R}} \pi^{-1}\tfrac{\epsilon}{(\lambda-\nu)^2+\epsilon^2}C_1\mathrm{d}E_0^{ac}(\nu)Q_n \\
&\qquad\qquad \times\int_{\mathbb{R}}\mathrm{d}E_0^{ac}(\eta)(C_2 - V_1(K_{1,n}-\eta-i\delta)^{-1}C_2).
\end{aligned}$$

Again, we insert the spectral representations and obtain

$$\begin{aligned}
&\int_{\mathbb{R}} \pi^{-1}\tfrac{\epsilon}{(\lambda-\nu)^2+\epsilon^2}C_1\mathrm{d}E_0^{ac}(\nu)Q_n\int_{\mathbb{R}}\mathrm{d}E_0^{ac}(\eta)(C_2 - V_1(K_{1,n}-\eta-i\delta)^{-1}C_2) \\
&\quad = \int_{\mathbb{R}} \pi^{-1}\tfrac{\epsilon}{(\lambda-\nu)^2+\epsilon^2}\sqrt{Y_1(\nu)}\check{Q}(\nu)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\nu))(\Phi_{K_0}\Phi_{2,0}^*)(\nu)\sqrt{Y_{2,0}(\nu)} \\
&\qquad - \int_{\mathbb{R}} \pi^{-1}\tfrac{\epsilon}{(\lambda-\nu)^2+\epsilon^2}\sqrt{Y_1(\nu)}\check{Q}(\nu)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\nu))\sqrt{Y_1(\nu)}Z_1C_1(K_{1,n}-\nu-i\delta)^{-1}C_2.
\end{aligned}$$

The limit of $C_1(K_{1,n}-\nu-i\delta)^{-1}C_2$ as $\delta\to+0$ exists in the Hilbert-Schmidt and the convergence is uniform in $\lambda\in\Lambda_n^\varphi$ by Proposition 5.2.2. Taking the limit and summing up the terms, taking into account the definition (5.30) of $G_{0,n}$, proves the lemma. □

Now we can calculate the final term $\Sigma_3(\epsilon,\delta,n)$ in the decomposition of the flux (5.18).

Lemma 5.2.16. *We have*

$$\begin{aligned}
&\lim_{n\to\infty}\lim_{\epsilon\to+0}\lim_{\delta\to+0}\Im\mathrm{m}\big[\mathrm{Tr}\big(\varrho_0\Sigma_3(\epsilon,\delta,n)\big)\big] \\
&\quad = -\pi\int_{\mathbb{R}}\mathrm{d}\lambda\mathrm{Tr}\Big(\check{\varrho}_0(\lambda)\big(\check{W}_{1,-}^*(\lambda)\check{T}_2^*(\lambda)\check{W}_{1,+}(\lambda)\check{Q}(\lambda)\check{T}_1(\lambda) \\
&\qquad\qquad + \check{T}_1^*(\lambda)\check{Q}(\lambda)\check{W}_{1,+}^*(\lambda)\check{T}_2(\lambda)\check{W}_{1,-}(\lambda)\big)\Big).
\end{aligned} \tag{5.39}$$

Proof. The scheme is the same as in the proof of Lemma 5.2.14 for Σ_4, but we have to treat the two summands of $\Sigma_3(\epsilon,\delta,n)$ simultaneously to be able to calculate the imaginary part. Recall that

$$\begin{aligned}
\Sigma_3(\epsilon,\delta,n) = &-W_{1,-}^*(n)V_1P_0^{ac}Q_n\widetilde{W}_{2,-}(\epsilon,n)W_{1,-}(n) \\
&- W_{1,-}^*(n)\big(W_{2,-}^*(\epsilon,n)V_2W_{1,+}(\delta,n) + F^*(\epsilon,\delta,n)\big)Q_n\widetilde{W}_{1,-}(n).
\end{aligned}$$

Using (5.34), we get

$$\begin{aligned}
&W_{1,-}^*(n)\big(W_{2,-}^*(\epsilon,n)V_2W_{1,+}(\delta)+F^*(\epsilon,\delta,n)\big)Q_n\widetilde{W}_{1,-}(n)\\
&\quad=\lim_{\varepsilon\to+0}W_{1,-}^*(n)\int_{\mathbb{R}}\mathrm{d}E_{K_1}(\gamma)P_1(\Lambda_n)C_2J_{2,n}(\gamma-i\epsilon)C_2\big(1-(K_{1,n}-\gamma+i\epsilon)^{-1}V_1\big)\\
&\qquad\qquad\times Q_n\int_{\mathbb{R}}(K_{0,n}-\eta-i\varepsilon)^{-1}C_1^*J_{1,n}(\eta+i\varepsilon)C_1P_{0,n}^{ac}\mathrm{d}E_0^{ac}(\eta).
\end{aligned}$$

Similarly, we obtain

$$\begin{aligned}
&\lim_{\epsilon\to+0}W_{1,-}^*(n)V_1P_0^{ac}Q_n\widetilde{W}_{2,-}(\epsilon,n)W_{1,-}(n)\\
&\quad=\lim_{\epsilon\to+0}\lim_{\varepsilon\to+0}\int_{\mathbb{R}}\mathrm{d}E_0^{ac}(\gamma)C_1^*J_{1,n}(\gamma-i\varepsilon)C_1P_0^{ac}Q_n\int_{\mathbb{R}}(K_{0,n}-\eta-i\epsilon)^{-1}\\
&\qquad\qquad\times(1-V_1(K_{1,n}-\eta-i\epsilon)^{-1})C_2J_{2,n}(\eta+i\epsilon)C_2\mathrm{d}E_{K_1}(\eta)W_{1,-}(n).
\end{aligned}$$

Again, we pass to the spectral representation and get an integral operator. Namely,

$$\begin{aligned}
&\Big(\Phi_{K_0}W_{1,-}^*(n)\big(W_{2,-}^*(\epsilon,n)V_2W_{1,+}(\delta,n)+F^*(\epsilon,\delta,n)\big)Q_n\widetilde{W}_{1,-}(\varepsilon)\Phi_{K_0}^*\check{f}\Big)(\lambda)\\
&\quad=\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\check{W}_{1,-}^*(\lambda)\sqrt{Y_2(\lambda)}J_{2,n}(\lambda-i\epsilon)\int_{\mathbb{R}}\mathrm{d}\xi\,G_{\epsilon,n}^*(\lambda,\xi)\check{Q}(\xi)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\xi))\\
&\qquad\times\int_{\mathbb{R}}\mathrm{d}\eta\,(\xi-\eta-i\varepsilon)^{-1}\sqrt{Y_1(\xi)}J_1(\eta+i\varepsilon)\sqrt{Y_1(\eta)}\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\eta))\check{f}(\eta)
\end{aligned}$$

for $\check{f}\in L^2(\mathbb{R},\mathrm{d}\lambda,\mathfrak{H}_\lambda)$. Similarly,

$$\begin{aligned}
&\Big(\Phi_{K_0}W_{1,-}^*(\varepsilon)V_1P_0^{ac}Q_n\widetilde{W}_{2,-}(\epsilon,n)W_{1,-}(n)\Phi_{K_0}^*\check{f}\Big)(\lambda)\\
&\quad=\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\sqrt{Y_1(\lambda)}J_{1,n}(\lambda-i\delta)\int_{\mathbb{R}}\mathrm{d}\xi\,\sqrt{Y_1(\xi)}\check{Q}(\xi)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\xi))\int_{\mathbb{R}}\mathrm{d}\eta\\
&\qquad\times(\xi-\eta-i\epsilon)^{-1}G_{\epsilon,n}(\eta,\xi)J_{2,n}(\eta+i\epsilon)\sqrt{Y_2(\eta)}\check{W}_{1,-}(\eta)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\eta))\check{f}(\eta).
\end{aligned}$$

We calculate the traces and obtain

$$\begin{aligned}
&\mathrm{Tr}\big(\varrho_0W_{1,-}^*(n)\big(W_{2,-}^*(\epsilon,n)V_2W_{1,+}(\delta,n)+F^*(\epsilon,\delta,n)\big)Q_n\widetilde{W}_{1,-}(\varepsilon,n)\big)\\
&\quad=\int_{\mathbb{R}}\mathrm{d}\lambda\,\mathrm{Tr}\Big(\check{\varrho}_0(\lambda)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\check{W}_{1,-}^*(\lambda)\sqrt{Y_2(\lambda)}J_{2,n}(\lambda-i\epsilon)\int_{\mathbb{R}}\mathrm{d}\xi\,G_{\epsilon,n}^*(\lambda,\xi)\\
&\qquad\times\check{Q}(\xi)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))(\xi-\lambda-i\varepsilon)^{-1}\sqrt{Y_1(\xi)}J_{1,n}(\lambda+i\varepsilon)\sqrt{Y_1(\lambda)}\Big)
\end{aligned}\tag{5.40}$$

and

$$\begin{aligned}
&\mathrm{Tr}\big(\varrho_0W_{1,-}^*(\varepsilon,n)V_1P_0^{ac}Q_n\widetilde{W}_{2,-}(\epsilon,n)W_{1,-}(n)\Phi_{K_0}^*\big)\\
&\quad=\int_{\mathbb{R}}\mathrm{d}\lambda\,\mathrm{Tr}\Big(\sqrt{Y_1(\lambda)}J_{1,n}(\lambda-i\varepsilon)\int_{\mathbb{R}}\mathrm{d}\xi\,\sqrt{Y_1(\xi)}\check{Q}(\xi)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\xi))\\
&\qquad\times(\xi-\lambda-i\epsilon)^{-1}G_{\epsilon,n}(\lambda,\xi)J_{2,n}(\lambda+i\epsilon)\sqrt{Y_2(\lambda)}\check{W}_{1,-}(\lambda)\Big).
\end{aligned}\tag{5.41}$$

Observe that the adjoint of (5.40) matches (5.41) except that $-i\epsilon$ in $(\xi-\lambda-i\epsilon)^{-1}$ is

replaced by $+i\varepsilon$ and vice versa. Using this, we obtain

$$\begin{aligned}
&\lim_{\epsilon\to+0}\Im\mathrm{m}\Big[\mathrm{Tr}\Big(\varrho_0 W_{1,-}^*(n)(W_{2,-}^*(\epsilon,n)V_2W_{1,+}(\delta)+F^*(\epsilon,\delta,n))Q_n\widetilde{W}_{1,-}(n)\\
&\qquad\qquad+\varrho_0 W_{1,-}^*(n)V_1P_0^{ac}Q_n\widetilde{W}_{2,-}(\epsilon,n)W_{1,-}(n)\Big)\Big]\\
&=\lim_{\epsilon\to+0}\lim_{\varepsilon\to+0}\int_{\mathbb{R}}\mathrm{d}\lambda\mathrm{Tr}\Big(\check{\varrho}_0(\lambda)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\Big(\check{W}_{1,-}^*(\lambda)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\sqrt{Y_2(\lambda)}\\
&\qquad\times J_{2,n}(\lambda-i\epsilon)\int_{\mathbb{R}}\mathrm{d}\xi\,G_{\epsilon,n}^*(\lambda,\xi)\check{Q}(\xi)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\xi))\\
&\qquad\times\big((\xi-\lambda-i\varepsilon)^{-1}-(\xi-\lambda+i\epsilon)^{-1}\big)\sqrt{Y_1(\xi)}J_{1,n}(\lambda+i\epsilon)\sqrt{Y_1(\lambda)}\\
&\quad+\sqrt{Y_1(\lambda)}J_{1,n}(\lambda-i\epsilon)\int_{\mathbb{R}}\mathrm{d}\xi\,\sqrt{Y_1(\xi)}\check{Q}(\xi)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\xi))(2i)^{-1}\\
&\quad\times\big((\xi-\lambda-i\epsilon)^{-1}-(\xi-\lambda+i\varepsilon)^{-1}\big)G_{\epsilon,n}(\lambda,\xi)J_{2,n}(\lambda+i\epsilon)\sqrt{Y_2(\lambda)}\check{W}_{1,-}(\lambda)\Big)\Big)\\
&=\pi\int_{\mathbb{R}}\mathrm{d}\lambda\mathrm{Tr}\Big(\check{\varrho}_0(\lambda)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\check{W}_{1,-}^*(\lambda)\Big(\sqrt{Y_2(\lambda)}J_2(\lambda-i0)G_0^*(\lambda,\lambda)\check{Q}(\lambda)\\
&\qquad\qquad\times\sqrt{Y_1(\lambda)}J_1(\lambda+i0)\sqrt{Y_1(\lambda)}\\
&\quad+\sqrt{Y_1(\lambda)}J_1(\lambda-i0)\sqrt{Y_1(\lambda)}\check{Q}(\lambda)G_0(\lambda,\lambda)J_2(\lambda+i0)\sqrt{Y_2(\lambda)}\check{W}_{1,-}(\lambda)\Big)\Big).
\end{aligned}$$

We made use of the fact that the limit in the trace is uniform in λ for $\lambda\in\Lambda_n$ and that

$$\int_{\mathbb{R}}\mathrm{d}\xi(\xi-\lambda-i\delta)^{-1}X(\xi)=\int_{|\xi-\lambda|\geq\delta}\mathrm{d}\xi(\xi-\lambda)^{-1}X(\xi)+i\pi X(\lambda)$$

for $X\in L^2(\mathbb{R},\mathfrak{L}_2(\mathfrak{H}))$ by Lemma A.2.20. Using Lemma 5.2.15 gives us

$$\begin{aligned}
&\lim_{\epsilon\to+0}\Im\mathrm{m}\Big[\mathrm{Tr}\Big(\varrho_0 W_{1,-}^*(n)W_{2,-}^*(\epsilon,n)V_2W_{1,+}(\delta,n)+F^*(\epsilon,\delta,n))Q_n\widetilde{W}_{1,-}(n)\\
&\qquad\qquad+W_{1,-}^*(n)V_1P_0^{ac}Q_n\widetilde{W}_{2,-}(\epsilon,n)W_{1,-}(n)\Big)\Big]\\
&=\pi\int_{\Lambda_n}\mathrm{d}\lambda\mathrm{Tr}\Big(\check{\varrho}_0(\lambda)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\Big(\check{W}_{1,-}^*(\lambda)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\sqrt{Y_2(\lambda)}J_{2,n}(\lambda-i0)\\
&\qquad\times\sqrt{Y_2(\lambda)}\check{W}_{1,+}(\lambda)\check{Q}(\lambda)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\sqrt{Y_1(\lambda)}J_{1,n}(\lambda+i0)\sqrt{Y_1(\lambda)}\\
&\quad+\sqrt{Y_1(\lambda)}J_{1,n}(\lambda-i0)\sqrt{Y_1(\lambda)}\check{Q}(\lambda)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\check{W}_{1,+}^*(\lambda)\\
&\qquad\times\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\sqrt{Y_2(\lambda)}J_{2,n}(\lambda+i0)\sqrt{Y_2(\lambda)}\check{W}_{1,-}(\lambda)\Big)\Big)\\
&=\pi\int_{\mathbb{R}}\mathrm{d}\lambda\mathrm{Tr}\Big(\check{\varrho}_0(\lambda)\mathcal{M}(\chi_{\Lambda_n^\varphi(\mu)}(\lambda))\Big(\check{W}_{1,-}^*(\lambda)\check{T}_2^*(\lambda)\check{W}_{1,+}(\lambda)\check{Q}(\lambda)\check{T}_1(\lambda)\\
&\qquad\qquad+\check{T}_1^*(\lambda)\check{Q}(\lambda)\check{W}_{1,+}^*(\lambda)\check{T}_2(\lambda)\check{W}_{1,-}(\lambda)\Big)\Big).
\end{aligned}$$

We can take the limit $n \to \infty$ and obtain

$$\begin{aligned}
&\lim_{n\to\infty}\lim_{\epsilon\to+0} -\Im\mathrm{m}\Big[\mathrm{Tr}\Big(\varrho_0 W_{1,-}^*(n)W_{2,-}^*(\epsilon,n)V_2W_{1,+}(\delta,n) + F^*(\epsilon,\delta,n))Q_n\widetilde{W}_{1,-}(n) \\
&\qquad\qquad + W_{1,-}^*(n)V_1P_0^{ac}Q_n\widetilde{W}_{2,-}(\epsilon,n)W_{1,-}(n)\Big)\Big] \\
&= -\pi\int_{\mathbb{R}}\mathrm{d}\lambda\mathrm{Tr}\Big(\check{\varrho}_0(\lambda)\Big(\check{W}_{1,-}^*(\lambda)\check{T}_2^*(\lambda)\check{W}_{1,+}(\lambda)\check{Q}(\lambda)\check{T}_1(\lambda) \\
&\qquad\qquad + \check{T}_1^*(\lambda)\check{Q}(\lambda)\check{W}_{1,+}^*(\lambda)\check{T}_2(\lambda)\check{W}_{1,-}(\lambda)\Big)\Big).
\end{aligned}$$

□

Theorem 5.1.8 follows easily from Lemmas 5.2.10, 5.2.11, 5.2.14, and 5.2.16. We only have to sum up (5.22), the imaginary part of (5.25), (5.33), and (5.39) to get

$$\begin{aligned}
&\lim_{n\to\infty}\mathfrak{J}_Q(n) \\
&= -2\int_{\mathbb{R}}\mathrm{d}\lambda\mathrm{Tr}\Big(\Im\mathrm{m}[\check{\varrho}_0(\lambda)\check{T}_1^*(\lambda)\check{Q}(\lambda)] - \pi\check{\varrho}_0(\lambda)\check{T}_1^*(\lambda)\check{Q}(\lambda)\check{T}_1(\lambda) \\
&\qquad + \Im\mathrm{m}[\check{\varrho}_0(\lambda)\check{W}_{1,-}^*(\lambda)\check{T}_2^*(\lambda)\check{W}_{1,+}(\lambda)\check{Q}(\lambda)] \\
&\qquad - \pi\check{\varrho}_0(\lambda)\check{W}_{1,-}^*(\lambda)\check{T}_2^*(\lambda)\check{W}_{1,+}(\lambda)\check{Q}(\lambda)\check{T}_1(\lambda) \\
&\qquad - \pi\check{\varrho}_0(\lambda)\check{T}_1(\lambda)\check{Q}(\lambda)\check{W}_{1,+}^*(\lambda)\check{T}_2(\lambda)\check{W}_{1,-}(\lambda) \\
&\qquad - \pi\check{\varrho}_0(\lambda)\check{W}_{1,-}^*(\lambda)\check{T}_2^*(\lambda)\check{W}_{1,+}(\lambda)\check{Q}(\lambda)\check{W}_{1,+}^*(\lambda)\check{T}_2(\lambda)\check{W}_{1,-}(\lambda)\Big) \\
&= -2\int_{\mathbb{R}}\mathrm{d}\lambda\mathrm{Tr}\Big(\Im\mathrm{m}[\check{\varrho}_0(\lambda)\check{T}^*(\lambda)\check{Q}(\lambda)] - \pi\check{\varrho}_0(\lambda)\check{T}^*(\lambda)\check{Q}(\lambda)\check{T}(\lambda)\Big),
\end{aligned}$$

where we used $T = T_1 + W_{1,+}^*T_2W_{1,-}$. This concludes the proof of Theorem 5.1.8.

5.3 The 1-photon Pauli-Fierz quantum dot LED

We want to model a QD-LED that can emit photons of arbitrary energy. As in the previous chapter, we have a small quantum system S contacted by a left lead l and a right lead r. The quantum system is based on the one-dimensional 1-photon Pauli-Fierz model of Section 2.2. Recall once more the essentials of our modeling approach as stated in the introductory Section 1.2. The electron together with its photon field is considered to be a single fermionic particle in the sense of the Landauer-Büttiker formalism, whence we work with the single-particle Hilbert space $\mathfrak{h}^{el} \otimes \mathfrak{h}^{ph}$. In this section we use the 1-photon Pauli-Fierz model, which implies that $\mathfrak{h}^{ph} = \mathbb{C} \oplus L^2(\mathbb{R}, \mathrm{d}k)$ is the space of at most one photon. The modeling assumption behind the 1-photon simplification is that every electron can emit at most one photon when passing through the quantum system. If we consider a system where all except two of the eigenvalues of the electron quantum system lie above the maximum of the chemical potentials, this appears to be a reasonable simplification. Again, we stress that we have infinitely many copies of the 'single particle' in the Landauer-Büttiker formalism. This implies that although the single-particle Hilbert space contains at most one photon, we can indeed use the 1-photon Pauli-Fierz model to describe arbitrarily many photons with the help

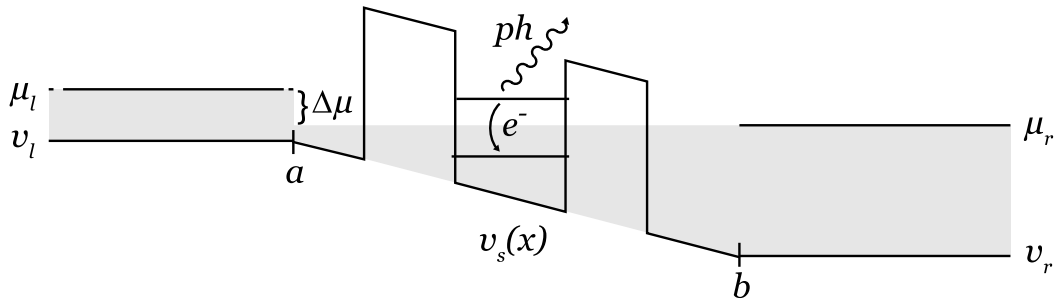

Figure 5.1: Pauli-Fierz QD-LED with double barrier potential

of a density operator. The electrons are now no longer labeled by the amount of photons, but by the continuous photon momentum $k \in \mathbb{R}$.

We start the description of the model with the electron part before adding the photons and their interaction. The electron model is taken from [8]. The electron Hilbert space is $\mathfrak{h}^{el} = L^2(\mathbb{R}, \mathrm{d}x)$. The Hilbert spaces of the left lead l and the right lead r are $\mathfrak{h}_l^{el} = L^2((-\infty, a], \mathrm{d}x)$ and $\mathfrak{h}_r^{el} = L^2([b, \infty), \mathrm{d}x)$, respectively. The Hilbert space of the quantum system is $\mathfrak{h}_S^{el} = L^2((a, b), \mathrm{d}x)$. The projections onto $\mathfrak{h}_j^{el}$ are denoted by p_j^{el}, $j \in \{l, S, r\}$. The decoupled electron system is described by $h_0^{el} = h_l^{el} \oplus h_S^{el} \oplus h_r^{el}$. Here,

$$h_j^{el} = -\tfrac{\mathrm{d}^2}{\mathrm{d}x^2} + \mathcal{M}(v_j(x)), \qquad j \in \{l, S, r\},$$

where $v_l(x) = v_l \in \mathbb{R}$, $v_r(x) = v_r \in \mathbb{R}$ with $v_r < v_l$, $v_S \in L^\infty\big((a, b), \mathrm{d}x\big)$, and we take homogeneous Dirichlet boundary conditions at a and b for the second derivative, i.e.

$$\mathrm{dom}(h_0^{el}) = \{f_{el} \in W^{2,2}(\mathbb{R}) \,|\, f_{el}(a) = f_{el}(b) = 0\}.$$

The coupled electron system is described by $h^{el} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \mathcal{M}(v(x))$ with domain $\mathrm{dom}(h^{el}) = W^{2,2}(\mathbb{R})$, where we define $v(x) = v_l(x) \oplus v_S(x) \oplus v_r(x)$. We assume that v_S is such that h^{el} is absolutely continuous (e.g. $v_S > v_r$). The free photon Hamiltonian

$$h^{ph} = \begin{pmatrix} 0 & 0 \\ 0 & \mathcal{M}(\omega(k)) \end{pmatrix}$$

acts on the Hilbert space $\mathfrak{h}^{ph} = \mathfrak{h}_0^{ph} \oplus \mathfrak{h}_1^{ph}$ with $\mathfrak{h}_0^{ph} = \mathbb{C}\Omega$ and $\mathfrak{h}_1^{ph} = L^2(\mathbb{R}, \mathrm{d}k)$. Its domain is

$$\mathrm{dom}(h^{ph}) = \Big\{(f_{ph}^{(0)}, f_{ph}^{(1)}) \in \mathfrak{h}^{ph} \,\Big|\, \int_{\mathbb{R}} \mathrm{d}k \, |\omega(k) f_{ph}^{(1)}(k)|^2 < \infty\Big\}.$$

Recall that the electron-photon interaction is given by

$$V_{int} = \begin{pmatrix} 0 & \langle G| \\ |G\rangle & 0 \end{pmatrix} \tag{5.42}$$

on $L^2((a,b),\mathrm{d}x)\oplus L^2((a,b)\times\mathbb{R},\mathrm{d}x\times\mathrm{d}k)$, where

$$\langle G(x)|:\mathfrak{h}_1^{ph}\to\mathbb{C},\qquad (\langle G(x)|f_1^{ph})(k)=\int_{\mathbb{R}}\mathrm{d}k\,\overline{G(x,k)}f_1^{ph}(k)$$

with $G(x,k)=e^{ikx}\omega(k)^{-\frac{1}{2}}\kappa(|k|)$, $\kappa\in C_0^\infty(\mathbb{R}_+)$, for $x\in(a,b)$ and $|G(x)\rangle=\langle G(x)|^*$. We extend (5.42) to

$$\mathfrak{H}=\mathfrak{h}^{el}\otimes\mathfrak{h}^{ph}=L^2(\mathbb{R},\mathrm{d}x)\oplus L^2(\mathbb{R}^2,\mathrm{d}x\times\mathrm{d}k)$$

by continuation with zero for $x\notin(a,b)$. We obtain the Hamiltonian H_0 with decoupled leads and no electron-photon interaction

$$H_0=h_0^{el}\otimes I_{ph}+I_{el}\otimes h^{ph}. \tag{5.43}$$

If we couple the leads to the quantum system, we get the Hamiltonian

$$H_{el}=h^{el}\otimes I_{ph}+I_{el}\otimes h^{ph} \tag{5.44}$$

The final Hamiltonian of the total system with coupled leads and electron-photon interaction is

$$H_{ph}=h^{el}\otimes I_{ph}+I_{el}\otimes h^{ph}+\tau_{int}V_{int}. \tag{5.45}$$

We know from [8] that h_0^{el} and h^{el} are densely defined, bounded from below self-adjoint operators. h^{ph} is obviously also a densely defined, bounded from below self-adjoint since $\omega(k)\geq 0$ for every $k\in\mathbb{R}$. It follows that H_0 and H_{el} are densely defined, bounded from below self-adjoint operators on $\mathfrak{H}$ with domains

$$\mathrm{dom}(H_0)=\mathrm{clo}_{\|\cdot\|_{H_0}}(\mathrm{dom}(h_0^{el})\otimes\mathrm{dom}(h^{ph}))$$

and

$$\mathrm{dom}(H_{el})=\mathrm{clo}_{\|\cdot\|_{H_{el}}}(\mathrm{dom}(h^{el})\otimes\mathrm{dom}(h^{ph})),$$

where the tensor product is in this case an algebraic tensor product. Since V_{int} is obviously a bounded operator, H_{ph} is also a densely defined, bounded from below self-adjoint operator on $\mathrm{dom}(H_{ph})=\mathrm{dom}(H_{el})$.

To apply the Landauer-Büttiker formula of Section 5.1, we have to write this model in terms of multiplication operators. We already mentioned in the introduction that a spectral representation ϕ^{ph} of h^{ph} is given by $\phi^{ph}:\mathfrak{h}^{ph}\to L^2(\mathbb{R}_+^0,\mathrm{d}\mathfrak{m}(\mu),\mathbb{C}^2)$ and

$$(\phi^{ph}(f_0^{ph},f_1^{ph}))(\mu)=\begin{cases}(f_0^{ph},0) & \text{if } \mu=0,\\ (f_1^{ph}(\mu),f_1^{ph}(-\mu)) & \text{if } \mu>0,\end{cases}$$

where $\mathrm{d}\mathfrak{m}(\mu)=\mathrm{d}\mu+\delta(\mu)\mathrm{d}\mu$. Thus, the unitary transformation $\Phi_{ph}=I_{el}\otimes\phi^{ph}$ maps the Hamiltonians H_0 and H_{el} to multiplication operators on $L^2(\mathbb{R}_+^0,\mathrm{d}\mathfrak{m}(\mu),\mathfrak{h})$, where $\mathfrak{h}=\mathfrak{h}^{el}\otimes\mathbb{C}^2$. Namely,

$$(\Phi_{ph}H_0f)(\mu)=\begin{pmatrix}h_0^{el}+\mu & 0\\ 0 & h_0^{el}+\mu\end{pmatrix}f'(\mu),\qquad f'=\Phi_{ph}f,\qquad f\in\mathfrak{H}$$

and

$$(\Phi_{ph} H_{el} f)(\mu) = \begin{pmatrix} h^{el} + \mu & 0 \\ 0 & h^{el} + \mu \end{pmatrix} f'(\mu), \qquad f' = \Phi_{ph} f, \qquad f \in \mathfrak{H}.$$

The Hamiltonians h_0^{el} and h^{el} are bounded from below, but not necessarily positive. However, it is easy to see that the the flux in Definition 5.1.7 is invariant with respect to a shift of the Hamiltonians by a constant. Thus, the flux does not change if we work with $H_j + \theta$, $j \in \{0, el, ph\}$, for some $\theta > 0$ large enough. Hence, if we define

$$H'_j = \Phi_{ph}(H_j + \theta)\Phi_{ph}^*, \qquad j \in \{0, el, ph\},$$

we obtain positive densely defined self-adjoint multiplication operators $H'_0 = \mathcal{M}(H'_0(\mu))$ and $H'_{el} = \mathcal{M}(H'_{el}(\mu))$ with

$$H'_0(\mu) = h'_0 + \mu, \qquad H'_{el} = h'_{el} + \mu,$$

where $h'_0 = h_0^{el} + \theta$ and $h'_{el} = h_{el} + \theta$ are positive densely defined self-adjoint operator H'_{ph} acting on the Hilbert space $L^2(\mathbb{R}^0_+, \mathrm{d}\mathfrak{m}(\mu), \mathfrak{h})$. It remains to check the trace class conditions (A1) and (A2). It is well-known that $(h^{el} - i)^{-1} - (h_0^{el} - i)^{-1}$ is a two-dimensional operator. In particular, it is trace class, whence (A1) holds. Assumption (A2) holds by the following proposition.

Proposition 5.3.1. *We have*

$$V_{ph} = (H_{el} + \theta)^{-1} - (H_{ph} + \theta)^{-1} \in \mathfrak{L}_1(\mathfrak{H})$$

for $\theta > 0$ sufficiently large.

Proof. Note that

$$(H_{el} + \theta)^{-1} - (H_{ph} + \theta)^{-1} = \big(1 + (H_{ph} + \theta)^{-1} V_{ph}\big)(H_{el} + \theta)^{-1} V_{ph} (H_{el} + \theta)^{-1}. \quad (5.46)$$

Let $R_\perp(\theta) = (h^{el} \otimes I_{ph} + I_{el} \otimes \mathcal{M}(\omega(k)) + \theta)^{-1}$. Since

$$(H_{el} + \theta)^{-1} = \begin{pmatrix} (h^{el} + \theta)^{-1} & 0 \\ 0 & (h^{el} \otimes I_{ph} + I_{el} \otimes \mathcal{M}(\omega(k)) + \theta)^{-1} \end{pmatrix},$$

we have

$$(H_{el} + \theta)^{-1} V_{ph} (H_{el} + \theta)^{-1} = \begin{pmatrix} 0 & (h^{el} + \theta)^{-1} \langle G | R_\perp(\theta) \\ R_\perp(\theta) |G\rangle (h^{el} + \theta)^{-1} & 0 \end{pmatrix}.$$

Now,

$$\begin{aligned} |G\rangle (h^{el} + \theta)^{-1} &= |G\rangle \mathcal{M}\big(\chi_{(a,b)}(x)\big)(h^{el} + \theta)^{-1} \\ &= |G\rangle \mathcal{M}\big(\chi_{(a,b)}(x)\big)(-\tfrac{\mathrm{d}^2}{\mathrm{d}x^2} + \theta)^{-1} \mathcal{M}(v(x))(h^{el} + \theta)^{-1}. \end{aligned}$$

It is well-known that $\mathcal{M}\big(\chi_{(a,b)}(x)\big)(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \theta)^{-1}$ is a trace class operator. It follows that $R_\perp(\theta)|G\rangle(h^{el} + \theta)^{-1}$ and its adjoint $(h^{el} + \theta)^{-1}\langle G|R_\perp(\theta)$ are also trace class operators. Since $\big(1 + (H + \theta)^{-1} V_{ph}\big)$ is bounded, the lemma follows from (5.46). □

To apply the Landauer-Büttiker formula, it remains to specify an initial state and an observable satisfying (A3) respectively (A4). We already mentioned that it is convenient for the analysis of an LED to work with an initial state of total darkness, i.e. with no photons present. Similarly to the usual Landauer-Büttiker formula, the electrons in the leads are in equilibrium. Hence, let $\rho_j^{el} = f_{FD}(h_j^{el} + \theta - \mu_j)$ with chemical potentials $\mu_j \in \mathbb{R}$, $j \in \{l, S, r\}$, where we have the Fermi-Dirac distribution function $f_{FD}(\lambda) = (e^{\beta\lambda} + 1)^{-1}$ with inverse temperature $\beta > 0$. The initial electron state is $\rho_0^{el} = \rho_a^{el} \oplus \rho_S^{el} \oplus \rho_b^{el}$. It commutes with h_0^{el} by construction. The no-photon state is $\rho_0^{ph} = I_{\mathbb{C}} \oplus 0$, which commutes with h^{ph}. The initial state of the total system is then

$$\rho = \rho_0^{el} \otimes \rho_0^{ph}. \tag{5.47}$$

Note that

$$\rho' = \Phi_{ph}(\rho_0^{el} \otimes \rho_0^{ph})\Phi_{ph}^* = \mathcal{M}(\rho_0^{el}\delta(\mu)), \tag{5.48}$$

satisfies (A3) since it commutes with H_0' and the exponential decay of the Fermi-Dirac function implies that $\varrho_0 = (H_0 + \theta)^2\rho$ is bounded.

We are interested in the electron current and the photon production rate. The observable for the electron current is

$$Q_j = -p_j^{el} \otimes I_{ph}, \tag{5.49}$$

the number of electrons in lead $j \in \{l, r\}$, where the minus sign reflects the negative charge of the electrons. Note that $Q_j' = \Phi_{ph}(-p_j^{el} \otimes I_{ph})\Phi_{ph}^* = \mathcal{M}(-p_j^{el})$ satisfies (A4). The observable for the photon production rate is

$$Q_{ph} = p_{h_0^{el}}^{ac} \otimes (0 \oplus I_{\mathfrak{h}_1^{ph}}) = \begin{pmatrix} 0 & 0 \\ 0 & p_{h_0^{el}}^{ac} \end{pmatrix}, \tag{5.50}$$

the number of photons. Note that the choice of $p_{h_0^{el}}^{ac}$ instead of I_{el} is of a technical nature. Since the wave operators do not exist in the middle system, we can measure the flux only in the leads. Note that

$$Q_{ph}' = \Phi_{ph} \begin{pmatrix} 0 & 0 \\ 0 & p_{h_0^{el}}^{ac} \end{pmatrix} \Phi_{ph}^* = \mathcal{M}(p_{h_0^{el}}^{ac}\chi_{(0,\infty)}(\mu))$$

also satisfies (A4). Note that $\mathfrak{m}(0) = 1$, whence the interval $(0, \infty)$ in the above equation is an open interval. Now we can apply the abstract Landauer-Büttiker formula of Theorem 5.1.8. Note that the unitary transformation and the translation by θ that we applied to H_j to obtain H_j', $j \in \{0, el, ph\}$, do not change the scattering matrix $S(\lambda)$, whence we take $S(\lambda)$ to be the scattering matrix of the scattering system $\{H_0, H_{ph}\}$ with respect to a spectral representation Φ_{H_0} of H_0^{ac}. As usual, if $X \in \mathfrak{B}(\mathfrak{H})$ commutes with H_0, we write $(\Phi_{H_0}Xf)(\lambda) = X(\lambda)(\Phi_{H_0}f)(\lambda)$ for a.e. $\lambda \in \mathbb{R}$ and $f \in \mathfrak{H}$, cf. Lemma A.2.5 in the appendix. Similarly, if $X_{el} \in \mathfrak{B}(\mathfrak{H})$ commutes with H_{el}, we write $(\Phi_{H_{el}}Xf)(\lambda) = \widehat{X}(\lambda)(\Phi_{H_{el}}f)(\lambda)$ for some spectral representation $\Phi_{H_{el}}$ of H_{el}^{ac}. Applying Theorem 5.1.8 gives us formulae for the electron current and the photon production rate.

Theorem 5.3.2. *Let H_j, $j \in \{0, el, ph\}$, be given by (5.43)–(5.45). Let ρ be given by (5.47). Let Q_j, $j \in \{l, r\}$, and Q_{ph} be given by (5.49) and (5.50). Then the electron current is given by*

$$\mathfrak{J}_j = \frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{d}\lambda \mathrm{Tr}\Big(\rho(\lambda)(S^*(\lambda)Q_j(\lambda)S(\lambda) - Q_j(\lambda))\Big),$$

and the photon production rate is given by

$$\mathfrak{J}_{ph} = \frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{d}\lambda \mathrm{Tr}\Big(\rho(\lambda)(S^*(\lambda)Q_{ph}(\lambda)S(\lambda) - Q_{ph}(\lambda))\Big).$$

Note that in the case of the photon production rate, the observable Q_{ph} commutes with H_{el}, whence we can also use the scattering system $\{H_{el}, H_{ph}\}$ to calculate the photon production rate. The resolvent difference $(H_{ph} - i)^{-1} - (H_{el} - i)^{-1}$ is trace class, whence we satisfy the requirements of the original Landauer-Büttiker formula of Theorem 3.1.2 if we choose $\rho_{el} = W_-(H_{el}, H_0)\rho W_-^*(H_{el}, H_0)$ as initial state. We obtain

$$\widetilde{\mathfrak{J}}_{ph} = \frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{d}\lambda \mathrm{Tr}\Big(\widehat{\rho}_{el}(\lambda)(\widehat{S}_{ph}^*(\lambda)\widehat{Q}_{ph}(\lambda)\widehat{S}_{ph}(\lambda) - \widehat{Q}_{el}(\lambda))\Big),$$

where $\widehat{S}_{ph}(\lambda)$ is the scattering matrix of the scattering system $\{H_{el}, H_{ph}\}$. Recall the decomposition $\mathfrak{J}_{Q,\rho_0} = \mathfrak{J}_{Q,\rho_0}^{el} + \mathfrak{J}_{Q,\rho_0}^{ph}$ of the flux from Proposition 3.2.14. In addition to ρ_{el}, we also define $Q_{el} = W_+(H_{el}, H_0)QW_+^*(H_{el}, H_0)$ for $Q \in \{Q_l, Q_r, Q_{ph}\}$. With the exact same calculations as in the proof of Proposition 3.2.14, we get a similar decomposition of the flux.

Proposition 5.3.3. *Let the assumptions of Theorem 5.3.2 hold. Then for an observable $Q \in \{Q_l, Q_r, Q_{ph}\}$, we have the decomposition $\mathfrak{J}_Q = \mathfrak{J}_Q^{el} + \mathfrak{J}_Q^{ph}$, where the coupling-induced flux is given by*

$$\mathfrak{J}_Q^{el} = \frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{d}\lambda \mathrm{Tr}\Big(\rho(\lambda)(S_{el}^*(\lambda)Q(\lambda)S_{el}(\lambda) - Q(\lambda))\Big),$$

and the photon-induced flux is given by

$$\mathfrak{J}_Q^{ph} = \frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{d}\lambda \mathrm{Tr}\Big(\widehat{\rho}_{el}(\lambda)(\widehat{S}_{ph}^*(\lambda)\widehat{Q}_{el}(\lambda)\widehat{S}_{ph}(\lambda) - \widehat{Q}_{el}(\lambda))\Big).$$

Corollary 5.3.4. *Let the assumptions of Theorem 5.3.2 hold. Then the coupling-induced electron current is equal to the electron current in the purely electric case, i.e.*

$$\mathfrak{J}_j^{el} = -\frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{d}\lambda \mathrm{Tr}\Big(\rho_0^{el}(\lambda)(s_{el}^*(\lambda)p_j^{el}(\lambda)s_{el}(\lambda) - p_j^{el}(\lambda))\Big) = \mathfrak{J}_{p_j,\rho_0^{el}}. \tag{5.51}$$

Also, the coupling-induced photon production rate vanishes, i.e. $\mathfrak{J}_{ph}^{el} = 0$, and $\mathfrak{J}_{ph} = \widetilde{\mathfrak{J}}_{ph}$.

Proof. The first statement follows immediately from $Q_j = p_j^{el} \otimes I_{ph}$, $\rho = \rho_0^{el} \otimes (1 \oplus 0)$, and the fact that

$$\begin{aligned} W_\pm(H_{el}, H_0) &= \operatorname*{s-lim}_{t\to\pm\infty} e^{it(h^{el}\otimes I_{ph} + I_{el}\otimes h^{ph})} e^{-it(h_0^{el}\otimes I_{ph} + I_{el}\otimes h^{ph})} p^{ac}_{h_0^{el}} \otimes I_{ph} \\ &= W_\pm(h^{el}, h_0^{el}) \otimes I_{ph}, \end{aligned}$$

which implies $S_{el} = s_{el} \otimes I_{ph}$. The second statement $\mathfrak{J}_{ph}^{el} = 0$ follows from

$$\rho = \rho_0^{el} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \qquad Q_{ph} = p^{ac}_{h_0^{el}} \otimes \begin{pmatrix} 0 & 0 \\ 0 & I_{\mathfrak{h}_1^{ph}} \end{pmatrix},$$

and $S_{el} = s_{el} \otimes I_{ph}$. Finally, since $W_+(H_{el}, H_0) = W_+(h^{el}, h_0^{el}) \otimes I_{ph}$ and

$$Q_{ph} = p^{ac}_{h_0^{el}} \otimes (0 \oplus I_{\mathfrak{h}_1^{ph}}),$$

we have $\big(Q_{ph}\big)_{el} = Q_{ph}$, which implies $\mathfrak{J}_{ph} = \widetilde{\mathfrak{J}}_{ph}$. □

Let us analyze the consequences of Proposition 5.3.3 and Corollary 5.3.4. First note that since $(H_{ph} - i)^{-1} - (H_{el} - i)^{-1} \in \mathfrak{L}_1(\mathfrak{H})$, the photon-induced flux $\mathfrak{J}_Q^{ph}$ falls into the regime of the usual Landauer-Büttiker formula for relatively trace class perturbations, Theorem 3.1.2. Secondly, (5.51) reduces the coupling-induced electron current to the fiber $\mu = 0$. But $(h^{el} - i)^{-1} - (h_0^{el} - i)^{-1} \in \mathfrak{L}_1(\mathfrak{h}^{el})$, whence this current can also be calculated using the Landauer-Büttiker formula of Theorem 3.1.2. Recall that the flux in Definition 5.1.7 was not derived from fundamental principles as in Chapter 3. However, this reduction of the current and the photon production rate to Theorem 3.1.2 shows once more that the definition connects to the fundamental principles of quantum mechanics.

Furthermore, Proposition 5.3.3 and Corollary 5.3.4 also reduce the calculation of the scattering matrix to the calculation of s_{el} and S_{ph}. But the corresponding scattering systems $\{h_0^{el}, h^{el}\}$ and $\{H_{el}, H_{ph}\}$ are trace class, whence Theorem 4.1.14 applies, which gives a formula for the scattering matrix in terms of the Weyl function and an extension parameter. Note, however, that $S_{ph}(\lambda)$ is truly an infinite-dimensional operator, in contrast to the Jaynes-Cummings QD-LED, where the scattering matrix was finite-dimensional.

6 Conclusion

The production technology for semiconductor quantum devices has made considerable progress in the last decade, which makes the study of their optoelectronic properties highly relevant. The goal of this thesis was the modeling of a quantum dot LED as a small quantum system contacted by leads in which electrons can emit and absorb photons. We wanted to formulate the calculation of the electric current and the light production in the Landauer-Büttiker framework to obtain formulae for the electric current and the photon production rate that depend only on the initial state and the scattering matrix.

The crucial modeling idea that allowed us to fit a QD-LED into the Landauer-Büttiker formalism is the concept of individual photon fields for each electron, cf. Section 1.2. By considering an electron together with its photon field as a 'single particle' in the sense of the Landauer-Büttiker formalism, we eliminated the photon-induced electron-electron interaction. We justified this by making the assumption that the electron-photon interaction takes place only in the quantum dot region and the photons leave this area immediately. As in the usual Landauer-Büttiker formula, we also neglected the Coulomb interaction. As a result of this approach, it suffices to treat a single electron together with its photon field, rather than having to work on the full Fock space. However, these electrons are now labeled by the photons in their photon field, which implies that two electrons are no longer indistinguishable if they differ in the properties of their photon field.

The modeling of the electron-photon interaction is an important aspect. The physical model suggested by non-relativistic quantum electrodynamics is mathematically very difficult. This is why we looked for simpler models in Chapter 2. We presented the Jaynes-Cummings model and models of the Pauli-Fierz type, which still capture important features of the QD-LED, but are mathematically easier to handle.

As a first main result of this thesis, we gave a new proof of the Landauer-Büttiker formula for relatively trace class perturbations, Theorem 3.1.2, which we feel is more clear than the proof previously given by Aschbacher et al. [2]. It uses a special spectral representation that is constructed from the trace class perturbation. This abstract theorem was motivated by our QD-LED based on the Jaynes-Cummings model, which satisfies the assumptions of this abstract theorem. This model assumes that the quantum dot interacts only with a single mode of the electromagnetic field. We used one-dimensional semi-infinite lattices for the leads to obtain a simple coupling to the quantum dot. The application of the abstract Landauer-Büttiker formula to this model resulted in formulae for the electric current and the photon production rate, cf. Theorem 3.2.13. These formulae are consistent with what one expects for physical reasons, and the fluxes decompose into a part that is induced by the coupling of the leads to the sample and a part that is due to the electron-photon interaction. We gave two obvious choices for the initial state. If the initial state is $\rho_j = f_{FD}(H_j - \mu_j)$, $j \in \{l, r\}$, the Landauer-Büttiker formula for the electric current is formally identical to the usual formula in the purely

electric case, cf. Theorem 3.2.15. In particular, this implies that the current and the photon production rate vanish for equal chemical potentials. For $\widetilde{\rho}_j = f_{FD}(h_j^{el} - \mu_j) \otimes \rho^{ph}$, the initial steady state is not an equilibrium state for each subsystem, whence not all fluxes vanish at equal chemical potentials. Nevertheless, the coupling-induced part of the current is equal to the current in the purely electric case, cf. Proposition 3.2.16. In this case, the photon production rate can be positive even if there is no electric current, cf. Proposition 3.2.17. This is a consequence of the fact that the electrons can now be distinguished by the number of photons in their photon field, which allows them to relax into a lower energy state that is occupied by electrons with a different number of photons.

To compute the electric current and the photon production rate numerically in both models, it is necessary to compute the scattering matrices. In the purely electric case with two leads, the transition matrix $T(\lambda)$ is a 2×2-matrix resulting from a finite rank perturbation. However, in the case of the Jaynes-Cummings QD-LED, the resolvent difference is only trace class but not of finite rank, whence the formula for $T(\lambda)$ in terms of the Weyl function given by Behrndt et al. [12] does not apply. This is why we extended their result to the case of relatively trace class perturbations in Chapter 4. As a result, we obtained a formula for the transition matrix for relatively trace class scattering systems, which depends on the Weyl function and the extension parameter, cf. Theorem 4.1.14. We also constructed a boundary triplet for the Jaynes-Cummings QD-LED and applied the formula for the transition matrix. Since the fiber spaces $\mathfrak{h}(\lambda)$ are actually finite dimensional, this formula can be used to calculate the matrix elements of the transition matrix numerically. For a special choice of the coupling of the leads, we gave an explicit analytical calculation of the transition matrix.

The Jaynes-Cummings model contains only photons of a single fixed frequency. The Pauli-Fierz model, on the other hand, describes photons of arbitrary energy. This is why we constructed a model of a QD-LED based on a Pauli-Fierz model in Chapter 5. To be able to handle the scattering theory of this model, we restricted it to the subspace of at most one photon. As a result, the electron-photon interaction became a perturbation that is relatively trace class with respect to the Hamiltonian of the system with leads coupled to the sample. However, in this model the resolvent difference of the decoupled Hamiltonian and the Hamiltonian with coupled leads is an operator of multiplication on an L^2-space with a measure that has an absolutely continuous part. Hence, it is not trace class, but it is trace class in every fiber. This was the motivation for our third main result, a Landauer-Büttiker formula for two Hamiltonians that are multiplication operators with a trace class resolvent difference in the fiber, and a third Hamiltonian that is a relatively trace class perturbation of one of the multiplication operators, cf. Theorem 5.1.8. This formula extends the result for relatively trace class perturbations of Chapter 3. Thus, we obtained similar formulae for the electric current and the photon production rate of the Pauli-Fierz QD-LED as in the Jaynes-Cummings case, cf. Theorem 5.1.8. One result of the Landauer-Büttiker formula for the Pauli-Fierz QD-LED is a decomposition of the flux into a coupling-induced part and a photon-induced part, similar to the case of the Jaynes-Cummings QD-LED. This decomposition actually reduces the calculation of the electric current and the photon production rate to the trace class case. In particular, the Weyl function representation of the transition matrix also applies to the Pauli-Fierz QD-LED. However, the fiber spaces are truly infinite-dimensional in this case.

Finally, let us make some remarks on possible future work on this subject. A not much more complicated variant of the Jaynes-Cummings QD-LED is to use continuous leads living on $L^2(\mathbb{R}_\pm)$ instead of the semi-infinite discrete lattices we used in the present thesis. The coupling could be realized by connecting the endpoints of the continuous leads to the quantum dot in the framework of boundary triplets, where the coupling parameter B is provided by the Jaynes-Cummings QD-LED model with discrete leads, cf. Lemma 4.2.5.

An obvious improvement of the Pauli-Fierz QD-LED would be to allow an arbitrary initial state, not just darkness. One might use the fact that the photon production rate can be calculated using the Landauer-Büttiker formula for relatively trace class couplings of Chapter 3, cf. Corollary 5.3.4, to use a more general initial state than $\rho_0^{ph} = 1 \oplus 0$ as initial photon state when calculating the photon production rate. In particular, states of the form $\widetilde{\rho}_0^{ph} = \varrho^{ph}(h^{ph})$ are interesting, where $\varrho^{ph} : \mathbb{R}_+^0 \to [0,1]$ is a photon energy distribution such that

$$\int_0^\infty \mathrm{d}\mathfrak{m}(\mu)\, \varrho^{ph}(\mu) = 1.$$

This can be used to model the incident light in a solar cell. However, the total electron current is not well-defined for this choice of an initial state. Only the photon-induced part $\mathfrak{J}_j^{ph}$, $j \in \{l, r\}$, can be rigorously calculated. One might argue heuristically that the coupling induced electron current still has to be identical to the purely electric case and define the electron current as the sum of the purely electric current plus the well-defined photon-induced current. Although this is physically plausible, it places the definition of the electron current on the level of the Landauer-Büttiker formula and thus farther away from the fundamental principles of quantum mechanics. It would be of interest to find a more fundamental definition of the flux that is well-defined for such initial states and to prove a Landauer-Büttiker formula for this case. One possible approach for this is to approximate the photon Hamiltonian by a pure point Hamiltonian.

The extension of the Pauli-Fierz QD-LED to several or even arbitrarily many photons is certainly very relevant for many-level systems. Unfortunately, this is very difficult since one loses the trace class property of the electron-photon interaction. This makes the existence of the wave operators already an open question and even more so the definition of the flux and a Landauer-Büttiker formula.

A wide area of research is the numerical evaluation of the Landauer-Büttiker formulae for the electric current and the photon production rate. One can use the Weyl function formula of the scattering matrix, cf. Theorem 4.1.14, to numerically calculate the matrix elements of the transition matrix. This is essentially all that is needed to make numerical studies of the physical properties of the QD-LED and the influence of the different parameters on the fluxes. But the representation of the transition matrix is also useful to analytically investigate the behavior and properties of the QD-LED models. A second, different approach for the calculation of the scattering matrix is the Feshbach decomposition, which uses the decomposition of the unperturbed Hamiltonian H_0 into a block matrix, cf. Behrndt et al. [10].

All of the electron-photon interaction models that we use in this thesis are based on single-photon effects. It would be interesting to formulate models that include multi-photon effects like they might appear in quantum dot solar cells. If one wants to go beyond our modeling approach of every electron having its own photon field, one faces

very strong difficulties since it becomes much harder to avoid working in the second quantization. Nevertheless, this would be interesting since it would open up the possibility to include the Coulomb interaction and to analyze the effect of the photon-mediated electron-electron interaction.

In summary one can say that the calculation of current and light production in a QD-LED including all physical effects is an immensely difficult task and our results provide a significant step into this direction.

Appendix

For the convenience of the reader, we recollect some essentials of second quantization in this Appendix A.1. Furthermore, we give a short introduction into mathematical scattering theory and operator spectral integrals in Appendix A.2.

A.1 Second quantization

Second quantization uses the Hilbert space of a single particle to construct a new Hilbert space, the so-called Fock space, that is very well suited to quantum mechanical systems with an unknown or varying amount of particles. This includes a formalism to raise the single-particle Hamiltonian to the Fock space. The creation and annihilation operators on this Fock space provide us with a very convenient tool to formulate interactions between the particles. Since not every physical state that has infinitely many particles can be expressed in terms of the Fock space without difficulties, we also make use of the C^*-algebraic formulation of quantum mechanics.

The central reference for this part A.1 of the appendix is [15], a widely accepted standard book, in particular Sections 5.1 and 5.2. Most of the material presented here can be found in this work, although in a slightly different presentation, in particular with a stronger emphasis on the algebraic approach.

A.1.1 The Fock space

The usual L^2-space is not very useful for the description of a quantum system with varying particle numbers. To overcome this problem we start with a single particle Hilbert space and use it to construct a many-particle space, the Fock space.

Let $\mathfrak{h}$ be a Hilbert space. Then for $n \in \mathbb{N}$ we can define the Hilbert space $\mathfrak{F}(\mathfrak{h})$ as the direct sum of the n-fold tensor products of $\mathfrak{h}$, i.e.

$$\mathfrak{F}(\mathfrak{h}) = \bigoplus_{n \in \mathbb{N}_0} \mathfrak{h}^{\otimes n}, \qquad \mathfrak{h}^0 = \mathbb{C}\Omega.$$

This space is called the full *Fock space* of $\mathfrak{h}$. If we think of $\mathfrak{h}$ as the Hilbert space in which the states of a quantum mechanical particle live, the subspaces $\mathfrak{h}^{\otimes n}$ contain the states that describe n such particles. In particular, $\mathfrak{h}^0$ is the zero-particle space spanned by the *vacuum* Ω. In this sense the states in $\mathfrak{F}(\mathfrak{h})$ describe any number of identical particles. However, the space is too large since we know that quantum mechanical particles satisfy symmetry relations. Particles with identical properties can not be distinguished in quantum mechanics. This means that a 'permutation' of the particles, i.e. a permutation of the arguments of the wave function, does not change the properties of the system, i.e. the expectation values. For $g_1 \otimes \ldots \otimes g_n \in \mathfrak{h}^n$ and $g_{\tau(1)} \otimes \ldots \otimes g_{\tau(n)}$ to give identical

expectation values for all observables, they have to satisfy

$$g_1 \otimes \ldots \otimes g_n = \pm g_{\tau(1)} \otimes \ldots \otimes g_{\tau(n)}$$

for any permutation $\tau \in \mathcal{S}_n$, where $\mathcal{S}_n$ denotes the set of all permutations of n elements. The symmetry property, symmetric or anti-symmetric, is a property of the particle type. Particles like photons and gluons are symmetric with respect to their exchange and are called *bosons*. In contrast, electrons and quarks are anti-symmetric and called *fermions*. Hence, we define the *Bose-Fock space* $\mathfrak{F}_+(\mathfrak{h})$ (also 'bosonic Fock space') and the *Fermi-Fock space* $\mathfrak{F}_-(\mathfrak{h})$ (also 'fermionic Fock space') that are subspaces of $\mathfrak{F}(\mathfrak{h})$. We set

$$\mathfrak{F}_\pm(\mathfrak{h}) = \bigoplus_{n\in\mathbb{N}_0} \mathfrak{h}^{\otimes_\pm n}, \qquad \mathfrak{h}^{\otimes_\pm n} = \mathfrak{P}_\pm^{(n)} \mathfrak{h}^{\otimes n}, \tag{A.1.1}$$

with $\mathfrak{P}_\pm^{(n)}$ being defined through linear and continuous extension of $\mathfrak{P}_\pm^{(0)}\Omega = \Omega$,

$$\mathfrak{P}_+^{(n)} g_1 \otimes \ldots \otimes g_n = \frac{1}{n!} \sum_{\tau\in\mathcal{S}_n} g_{\tau(1)} \otimes \ldots \otimes g_{\tau(n)},$$

and

$$\mathfrak{P}_-^{(n)} g_1 \otimes \ldots \otimes g_n = \frac{1}{n!} \sum_{\tau\in\mathcal{S}_n} \operatorname{sgn}(\tau) g_{\tau(1)} \otimes \ldots \otimes g_{\tau(n)}$$

for $g_1, \ldots, g_n \in \mathfrak{h}$, $n \in \mathbb{N}$. The operators $\mathfrak{P}_\pm^{(n)}$ are orthogonal projections onto $\mathfrak{h}^{\otimes_\pm n}$, whence

$$\mathfrak{P}_\pm = \bigoplus_{n\in\mathbb{N}_0} \mathfrak{P}_\pm^{(n)}$$

is an orthogonal projection with range $\mathfrak{F}_\pm(\mathfrak{h})$. For convenience we introduce the dense subspace

$$\mathfrak{F}_\pm^{fin}(\mathfrak{h}) = \left\{ f \in \mathfrak{F}_\pm(\mathfrak{h}) \,|\, \exists\, N \in \mathbb{N} \,:\, f \in \textstyle\bigoplus_{n=0}^N \mathfrak{h}^{\otimes_\pm n} \right\}$$

of vectors with finite number of particles. Let us provide two interesting examples for a fermionic and bosonic Fock space.

Example A.1.1. *Consider the simplest possible single-particle Hilbert space, a space spanned by the single vector f. Note that $\mathfrak{P}_\pm \mathbb{C} f = \mathbb{C} f$. Obviously, $\mathfrak{P}_-^{(n)} f \otimes \ldots \otimes f = 0$ for $n > 1$. Thus, $\mathfrak{F}_-(\mathbb{C}) = \mathbb{C}^2 \cong \mathbb{C}\Omega \oplus \mathbb{C} f$. For the bosonic case note that $\mathbb{C}^{\otimes n} \cong \mathbb{C}$, whence $\mathfrak{F}_+(\mathbb{C}) = \ell^2(\mathbb{N}_0)$.*

Example A.1.2. *Now we choose $L^2(\mathbb{R})$ as the usual single-particle Hilbert space for a one-dimensional particle. Let $f_1, \ldots, f_n \in L^2(\mathbb{R})$. Then we can identify*

$$f_1(x_1) \otimes \ldots \otimes f_n(x_n) = \psi(x_1, \ldots, x_n), \qquad \psi \in L^2(\mathbb{R}^n).$$

In this sense $\mathfrak{P}_\pm^{(n)} f_1 \otimes \ldots \otimes f_n$ is a function that is symmetric (+) respectively anti-symmetric (−) in its variables $x_1, \ldots, x_n$. The spaces $\mathfrak{F}_\pm(L^2(\mathbb{R}))$ are then the Hilbert spaces spanned by all (anti-)symmetric square-integrable functions with an arbitrary number of variables.

We have created the Fock spaces $\mathfrak{F}_\pm(\mathfrak{h})$ from the single-particle space $\mathfrak{h}$. If all particles are independent, it should also be possible to obtain the observables of the many-particle system from the single-particle observables. Indeed, this is accomplished by the functor $\mathrm{d}\Gamma$. For any self-adjoint operator A on $\mathrm{dom}(A) \subset \mathfrak{h}$, let

$$\mathrm{d}\Gamma^{(n)}(A) = \sum_{j=1}^{n} I_\mathfrak{h} \otimes \ldots \otimes I_\mathfrak{h} \otimes \underset{\substack{\uparrow \\ j\text{-th position}}}{A} \otimes I_\mathfrak{h} \otimes \ldots \otimes I_\mathfrak{h}, \qquad \mathrm{d}\Gamma^{(0)}(A) = I_{\mathbb{C}\Omega}, \tag{A.1.2}$$

be defined on $\mathrm{dom}(A) \otimes \ldots \otimes \mathrm{dom}(A) \subset \mathfrak{h}^{\otimes n}$ (as algebraic tensor product) for $n \in \mathbb{N}$, and define

$$\mathrm{d}\Gamma(A) = \overline{\bigoplus_{n\in\mathbb{N}_0} \mathrm{d}\Gamma^{(n)}(A)}. \tag{A.1.3}$$

Lemma A.1.3. *Let A be a densely defined self-adjoint operator on the Hilbert space $\mathfrak{h}$. Then $\mathrm{d}\Gamma(A)$ defined by* (A.1.3) *leaves $\mathfrak{F}_\pm(A)$ invariant and is a densely defined self-adjoint operator on those spaces.*

Unitary operators U on $\mathfrak{h}$ are lifted to the Fock space using the functor Γ defined by

$$\Gamma(U) = \bigoplus_{n\in\mathbb{N}_0} \underbrace{U \otimes \ldots \otimes U}_{n \text{ times}}.$$

Lemma A.1.4. *For any two self-adjoint operators A, B on $\mathfrak{h}$, we have*

(i) $\Gamma(e^{itA}) = e^{it\mathrm{d}\Gamma(A)}$,

(ii) $\Gamma(AB) = \Gamma(A)\Gamma(B)$,

(iii) $\mathrm{d}\Gamma([A, B]) = [\mathrm{d}\Gamma(A), \mathrm{d}\Gamma(B)]$.

The operator $\mathrm{d}\Gamma(A)$ is often referred to as the *second quantization* of A. One special example is the second quantization of the identity. It is easy to check that

$$\mathfrak{N}_\pm : \mathrm{dom}(\mathfrak{N}) \subset \mathfrak{F}_\pm(\mathfrak{h}) \to \mathfrak{F}_\pm(\mathfrak{h}), \qquad \mathfrak{N}_\pm g^{(n)} = n g^{(n)}, \qquad g^{(n)} \in \mathfrak{h}_\pm^{\otimes n},$$

on the domain

$$\mathrm{dom}(\mathfrak{N}_\pm) = \Big\{ \{g^{(n)}\}_{n\in\mathbb{N}_0} \in \mathfrak{F}_\pm(\mathfrak{h}) \,\Big|\, \sum_{n\in\mathbb{N}_0} n^2 \|g^{(n)}\|^2 < \infty \Big\}$$

satisfies $\mathfrak{N}_\pm = \mathrm{d}\Gamma(I_{\mathfrak{F}_\pm(\mathfrak{h})})$. It is called the *number operator* since its eigenspaces are the n-particle subspaces $\mathfrak{h}^{\otimes_\pm n}$, $n \in \mathbb{N}_0$, and the eigenvalues are n, the number of particles.

A.1.2 The creation and annihilation operators

Obtaining the observables for the many-particle system from the single-particle observables is only possible if the individual particles are independent. To describe interacting particles, we need operators that do not factorize with respect to the tensor

product structure of the Fock space. A very convenient way to describe such operators are the creation and annihilation operators. For $f \in \mathfrak{h}$ we define the operators $a_\pm(f) : \mathrm{dom}(\mathfrak{N}_\pm^{\frac{1}{2}}) \to \mathfrak{F}_\pm(\mathfrak{h})$ by linear and continuous continuation of

$$a_\pm(f)\mathfrak{P}_\pm(g_1 \otimes g_2 \otimes \ldots \otimes g_n) = \sqrt{n}\left(\frac{1}{n}\sum_{j=1}^{n}\langle f, g_j\rangle\, \mathfrak{P}_\pm(g_2 \otimes \ldots \otimes g_{j-1} \otimes g_{j+1} \otimes \ldots \otimes g_n)\right) \tag{A.1.4}$$

and $a_\pm(f)\Omega = 0$ for $g_1, \ldots, g_n \in \mathfrak{h}$. Its adjoint is denoted by $a_\pm^*(f)$ and has the domain $\mathrm{dom}(a_\pm^*(f)) = \mathrm{dom}(a_\pm(f))$. It acts as

$$a_\pm(f)\mathfrak{P}_\pm(g_1 \otimes g_2 \otimes \ldots \otimes g_n) = \sqrt{n+1}\,\mathfrak{P}_\pm(f \otimes g_1 \otimes g_2 \otimes \ldots \otimes g_n), \qquad a_\pm(f)\Omega = f.$$

Note that if we interpret $f_1 \otimes \ldots \otimes f_n$ as the state with n particles in the states $f_1, \ldots, f_n$, then $f \otimes f_1 \otimes \ldots \otimes f_n$ describes $n+1$ particles in the states $f, f_1, \ldots, f_n$. Hence, the operator $a_\pm^*(f)$ creates a particle in the state f and is thus called *creation operator*. Its adjoint $a_\pm(f)$ annihilates a particle and is called *annihilation operator*. We call the operators $a_-(f)$ and $a_-^*(f)$ the *fermionic* annihilation and creation operators. Correspondingly, $a_+(f)$ and $a_+^*(f)$ are called *bosonic* annihilation and creation operators. Note that $\mathfrak{F}_\pm^{fin}(\mathfrak{h}) \subset \mathrm{dom}(a_\pm^\#(f))$ and $a_\pm^\#(f)\mathfrak{F}_\pm^{fin}(\mathfrak{h}) \subset \mathfrak{F}_\pm^{fin}$ for any $f \in \mathfrak{h}$. The creation and annihilation operators are particularly interesting because they are directly related to the second quantization of rank-one operators.

Lemma A.1.5. *Let $f, g \in \mathfrak{h}$. Then*

$$\mathrm{d}\Gamma(\langle g, \cdot\rangle f) = a_\pm^*(f)a_\pm(g).$$

In particular, this implies

$$\mathrm{d}\Gamma(A) = \sum_{j=1}^{\infty} a_\pm^*(f_j)a_\pm(g_j)$$

for any compact operator $A = \sum_{j=1}^{\infty}\langle g_j, \cdot\rangle f_j$ on $\mathfrak{h}$.

The canonical anti-commutation relations

In this section we give some details on the fermionic creation and annihilation operators. As we will see, they are easier to handle than their bosonic counterparts. To simplify notation we denote the fermionic annihilation operator by $b(f) = a_-(f)$ and the fermionic creation operator by $b^*(f) = a_-^*(f)$, $f \in \mathfrak{h}$. Let $[A, B]_- = AB + BA$ denote the anti-commutator. The following lemma states a very fundamental property of the fermionic annihilation and creation operators.

Lemma A.1.6. *The fermionic annihilation and creation operators satisfy the* canonical anti-commutation relations *(CAR)*

$$[b(f), b^*(g)]_- = \langle f, g\rangle, \qquad [b(f), b(g)]_- = [b^*(f), b^*(g)]_- = 0, \qquad f, g \in \mathfrak{h}. \tag{A.1.5}$$

An immediate consequence of these relations is that $b^{\#}(f)b^{\#}(f) = -b^{\#}(f)b^{\#}(f)$, where here and in the following $b^{\#}$ denotes either b or b^*. We obtain

$$b^*(f)b^*(f) = b(f)b(f) = 0. \tag{A.1.6}$$

This reflects the Pauli principle, which states that no two fermions may occupy the same state. Of course, this is caused by the anti-symmetrization projection $\mathfrak{P}_-$. Let $\sigma(\{1,\dots,j,\dots,k,\dots,n\}) = \{1,\dots,k,\dots,j\dots,n\}$ for some $j,k \in \{1,\dots,n\}$. Then

$$\begin{aligned}
&\mathfrak{P}_-(f_1 \otimes \dots \otimes f_j \otimes \dots \otimes f_k \otimes \dots \otimes f_n) \\
&\quad = \frac{1}{n!} \sum_{\substack{\tau\in\mathcal{S}_n \\ \mathrm{sgn}(\tau)=1}} f_{\tau(1)} \otimes \dots \otimes f_{\tau(j)} \otimes \dots \otimes f_{\tau(k)} \otimes \dots \otimes f_{\tau(n)} \\
&\qquad\quad -\frac{1}{n!} \sum_{\substack{\tau\in\mathcal{S}_n \\ \mathrm{sgn}(\tau)=1}} f_{\sigma(\tau(1))} \otimes \dots \otimes f_{\sigma(\tau(j))} \otimes \dots \otimes f_{\sigma(\tau(k))} \otimes \dots \otimes f_{\sigma(\tau(n))}
\end{aligned}$$

This sum is obviously zero if $f_j = f_k$. The CAR have a very important consequence.

Corollary A.1.7. *The fermionic annihilation and creation operators can be extended to bounded operators on $\mathfrak{F}_-(\mathfrak{h})$ with*

$$\|b(f)\| = \|b^*(f)\| = \|f\|, \qquad f \in \mathfrak{h}.$$

Proof. Using $b^*(f)b^*(f) = 0$, we have

$$(b^*(f)b(f))^2 = b^*(f)(b(f)b^*(f) + b^*(f)b(f))b(f) = \|f\|b^*(f)b(f)$$

on the dense subspace $\mathfrak{F}_-^{fin}(\mathfrak{h})$. Choose a $\psi \in \mathfrak{F}_-^{fin}(\mathfrak{h})$ such that $b^*(f)b(f)\psi \neq 0$. Then

$$\|b^*(f)b(f)\psi\|^2\langle\psi,(b^*(f)b(f))^2\psi\rangle = \langle\psi,\|f\|b^*(f)b(f)\psi\rangle \leq \|f\|^2\|\psi\|\|b^*(f)b(f)\psi\|,$$

whence $\|b^*(f)b(f)\psi\| \leq \|f\|^2\|\psi\|$. Thus, $\|b^*(f)b(f)\|$ is a bounded positive operator and it follows that $\|b(f)\| = \|b^*(f)\| = \|f\|$. □

Let us give two examples of fermionic creation and annihilation operators on the fermionic Fock spaces of $\mathbb{C}$ and $L^2(\mathbb{R})$, see Examples A.1.1 and A.1.2.

Example A.1.8. *Let the single-particle Hilbert space be $\mathfrak{h} = \mathbb{C}f$ with $\|f\| = 1$ as in Example A.1.1. Then $\mathfrak{F}_-(\mathfrak{h}) = \mathbb{C}\Omega \oplus \mathbb{C}f$ and since $\mathfrak{h}$ is one-dimensional, there is only one creation and one annihilation operator. Namely,*

$$b = b(f) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \qquad b^* = b^*(f) = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.$$

Note that

$$[b^*,b]_- = b^*b + bb^* = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = 1.$$

Example A.1.9. *Let $\mathfrak{h} = L^2(\mathbb{R})$ as in Example A.1.2. For $f \in \mathfrak{h}$ and $\psi \in \mathfrak{h}^{\otimes_- n}$, $n \in \mathbb{N}$, we have*

$$(b^*(f)\psi)(x_1, \ldots, x_{n+1}) = \frac{1}{n} \sum_{j=1}^{n} f(x_j)\psi(x_1, \ldots, x_{j-1}, x_{j+1}, \ldots, x_{n+1})$$

and

$$(b(f)\psi)(x_1, \ldots, x_{n-1}) = \sqrt{n} \int_{\mathbb{R}} \mathrm{d}x\, f(x)\psi(x, x_1, \ldots, x_{n-1}).$$

Note that the function ψ remains anti-symmetric after integrating out a variable, whence we do not have to anti-symmetrize again.

The canonical commutation relations

Let us now turn to the bosonic annihilation and creation operators. Again, we simplify notation by abbreviating $a(f) = a_+(f)$ and $a^*(f) = a_+^*(f)$. These operators also satisfy certain commutation relations.

Lemma A.1.10. *The bosonic annihilation and creation operators satisfy the* canonical commutation relations *(CCR)*

$$[a(f), a^*(g)] = \langle f, g\rangle, \qquad [a(f), a(g)] = [a^*(f), a^*(g)] = 0, \qquad f, g \in \mathfrak{h}.$$

It is important to note that $a(f)$ and $a^*(f)$ are unbounded operators. To give examples of bosonic annihilation and creation operators, let us consider once more the Fock spaces of Examples A.1.1 and A.1.2.

Example A.1.11. *Let $\mathfrak{h} = \mathbb{C}f$ with $\|f\| = 1$ as in Example A.1.1. Since $\mathfrak{h}$ is one-dimensional, we have only one annihilation operator $a = a(f)$ and one creation operator $a^* = a^*(f)$ on $\mathfrak{F}_+(\mathfrak{h}) = \ell^2(\mathbb{N}_0)$. Let $\{\Upsilon_n\}_{n\in\mathbb{N}_0}$ be an orthonormal basis of $\ell^2(\mathbb{N}_0)$ with $\mathfrak{h}^{\otimes_+ n} = \mathbb{C}\Upsilon_n$. Then*

$$a\Upsilon_{n+1} = \sqrt{n+1}\Upsilon_n, \qquad a^*\Upsilon_n = \sqrt{n+1}\Upsilon_{n+1}, \qquad n \in \mathbb{N}_0.$$

The annihilation and creation operators on $\mathfrak{F}_+(L^2(\mathbb{R}))$ are the same as in Example A.1.9 with $\mathfrak{P}_-$ replaced by $\mathfrak{P}_+$

Generalized annihilation and creation operators

If we consider a quantum system that does not contain only a single particle species, we can no longer work only on the Fock space. Let a fixed number of particles be described with the Hilbert space $\mathfrak{h}^1$, and let an infinite amount of other particles be given by the Fock space $\mathfrak{F}_\pm(\mathfrak{h}^2)$ with single-particle Hilbert space $\mathfrak{h}^2$. Then the whole system can be described with the Hilbert space $\mathfrak{h}^1 \otimes \mathfrak{F}_\pm(\mathfrak{h}^2)$. Of course, in this situation we still have the annihilation and creation operators $I_{\mathfrak{h}^1} \otimes a^\#(f)$, $f \in \mathfrak{h}^2$. However, if the annihilation and creation should depend on the other particle type, the operators can no longer respect the factorization of the tensor product structure. It is possible to generalize the notion of creation and annihilation operators on the Fock space to

spaces of the form $\mathfrak{h}^1 \otimes \mathfrak{F}_\pm(\mathfrak{h}^2)$. To this end we introduce a *form factor*, which is an operator $G \in \mathfrak{B}(\mathfrak{h}^1, \mathfrak{h}^1 \otimes \mathfrak{h}^2)$. It assumes the role of the states $\psi \in \mathfrak{F}_\pm(\mathfrak{h}^2)$ for which we can construct the usual annihilation and creation operators $a(\psi)$ and $a^*(\psi)$. For a form factor G we define the annihilation operator $(a(G))^{(n)}$ on $\mathfrak{h}^1 \otimes (\mathfrak{h}^2)^{\otimes_\pm n}$, $n \in \mathbb{N}$, by linear and continuous continuation of

$$\begin{aligned} &a_\pm^{(n)}(G)g \otimes (\mathfrak{P}_\pm^{(n)}\psi_1 \otimes \psi_2 \otimes \ldots \otimes \psi_n) \\ &\quad = \frac{1}{\sqrt{n}} \sum_{j=1}^{n} (G^*(g \otimes \psi_j)) \otimes (\mathfrak{P}_\pm^{(n-1)}\psi_1 \otimes \ldots \otimes \psi_{j-1} \otimes \psi_{j+1} \otimes \ldots \otimes \psi_n) \end{aligned}$$

for $g \in \mathfrak{h}^1$ and $\psi_1 \otimes \ldots \otimes \psi_n \in (\mathfrak{h}^2)^{\otimes_\pm n}$. It is easy to see that this operator is bounded with norm $\|a_\pm^{(n)}(G)\| = \sqrt{n}\|G\|$. The annihilation operator $a(G)$ on the full space $\mathfrak{h}^1 \otimes \mathfrak{F}_\pm(\mathfrak{h}^2)$ is defined by

$$a_\pm(G) = \bigoplus_{n \in \mathbb{N}_0} a^{(n)}(G), \quad a^{(0)}(G) = 0, \quad \mathrm{dom}(a(G)) = \Big\{ f \in \mathfrak{F}_\pm \,|\, \sum_{n \in \mathbb{N}_0} n\|f^{(n)}\|^2 < \infty \Big\}.$$

The adjoint operator is denoted by $a^*(G)$ and acts as

$$\begin{aligned} &(a^*)^{(n)}(G)g \otimes (\mathfrak{P}_\pm^{(n)}\psi_1 \otimes \psi_1 \otimes \ldots \otimes \psi_n) \\ &\quad = I_{\mathfrak{h}^1} \otimes \mathfrak{P}_\pm^{(n+1)}\sqrt{n+1}(Gg) \otimes (\psi_1 \otimes \psi_1 \otimes \ldots \otimes \psi_n) \in \mathfrak{h}^1 \otimes (\mathfrak{h}^2)^{\otimes_\pm (n+1)} \end{aligned}$$

for $n \in \mathbb{N}$, $g \in \mathfrak{h}^1$, and $\psi_1 \otimes \ldots \otimes \psi_n \in (\mathfrak{h}^2)^{\otimes_\pm n}$.

A.1.3 States as functionals on C*-algebras

It is well known that quantum mechanics can be formulated in an abstract framework using C^*-algebras. The objects in this language are the C^*-algebra of observables $\mathcal{A}$ and a normalized positive linear functional ϖ on $\mathcal{A}$ called the *state*. In the literature the states are usually denoted by ω, but we want to reserve this symbol for the dispersion relation of the photons in Chapters 2, 3, and 5. The relation to the traditional description of observables as operators on Hilbert spaces is obtained through the *Gelfand-Naimark-Segal construction*, which establishes a one-to-one correspondence up to unitary equivalence between cyclic representations and normalized positive linear functionals on $\mathcal{A}$. More precisely, for every state $\varpi : \mathcal{A} \to \mathbb{C}$ there exists a *GNS triplet* $(\pi_\varpi, \mathfrak{H}_\varpi, \Omega_\varpi)$ consisting of a cyclic representation π_ϖ on a Hilbert space $\mathfrak{H}_\varpi$ with cyclic vector Ω_ϖ such that $\varpi(A) = \langle \Omega_\varpi, A\Omega_\varpi \rangle$ for all $A \in \mathcal{A}$. With this construction one can realize any C^*-algebra as a subalgebra of $\mathfrak{B}(\mathfrak{H})$ for some Hilbert space $\mathfrak{H}$. Observables in quantum mechanics may in general be unbounded self-adjoint operators A. This can be incorporated into the C^*-algebra framework by working with the unitary group e^{itA}.

Let us now consider the so-called *CAR algebra* $\mathcal{A}_-(\mathfrak{h})$ for some Hilbert space $\mathfrak{h}$. It is the C^*-algebra generated by the elements $\{b(f) \,|\, f \in \mathfrak{h}\}$ that are anti-linear in f and satisfy the canonical anti-commutation relations (A.1.5). Since a state ϖ is continuous by definition and we have the CAR, it suffices to know the values of ϖ on the ordered monomials of the form $b^*(g_1) \cdots b^*(g_m) b(f_1) \cdots b(f_n)$, $g_j, f_k, \in \mathfrak{h}$, $1 \leq j \leq m$, $1 \leq k \leq n$, $m, n \in \mathbb{N}$, to know it by linearity and continuity on the whole algebra. It is physically

reasonable to demand that a state ϖ be gauge-invariant, i.e. invariant with respect to the unitary transformation U_θ on $\mathcal{A}_-(\mathfrak{h})$ given by $U_\theta b(f) = b(e^{i\theta}f)$. This simply means that expectation values do not change under a constant phase shift. Using the linearity of b^* and the anti-linearity of b, this immediately implies that

$$\varpi(b^*(g_1)\cdots b^*(g_m)b(f_1)\cdots b(f_n)) = e^{i(m-n)\theta}\varpi(b^*(g_1)\cdots b^*(g_m)b(f_1)\cdots b(f_n)),$$

which gives

$$\varpi(b^*(g_1)\cdots b^*(g_m)b(f_1)\cdots b(f_n)) = 0 \quad \text{if} \quad n \neq m.$$

An important subclass of gauge-invariant states are the quasi-free states. Physically speaking, these are states in which the individual particles do not interact with each other. This is reflected by the fact that ϖ is fully determined by the so-called two-point functionals $\varpi(a^*(f)a(g))$ for bosons and $\varpi(b^*(f)b(g))$ for fermions. To see this consider the expectation value $\varpi(b^*(f_1)b^*(f_2)b(g_1)b(g_2))$. It is the expectation value of the simultaneous transition of one fermion from g_1 to f_1 and another identical fermion from g_2 to f_2. Since the particles are indistinguishable, this is the same as the transitions $g_1 \rightsquigarrow f_2$ and $g_2 \rightsquigarrow f_1$, except for a minus sign from the fermionic character of the particles. Hence, one expects for non-interacting particles that

$$\begin{aligned}&\varpi(b^*(f_1)b^*(f_2)b(g_1)b(g_2))\\ &\quad = \varpi(b^*(f_1)b(g_1))\varpi(b^*(f_2)b(g_2)) - \varpi(b^*(f_1)b(g_2))\varpi(b^*(f_2)b(g_1)).\end{aligned}$$

The extension of this concept to $n \in \mathbb{N}$ particles results in the following definition.

Definition A.1.12. *We call a state on the CAR algebra* quasi-free *if it is gauge-invariant and*

$$\varpi(b^*(f_1)\cdots b^*(f_n)b(g_1)\ldots b(g_n)) = \det\left(\{\varpi(b^*(f_j)b(g_k))\}_{j,k=1}^n\right) \tag{A.1.7}$$

for all $f_j, g_j \in \mathfrak{h}$, $1 \leq j \leq n$, $n \in \mathbb{N}$.

Note that $\varpi(b^*(f)b(g))$ defines a bounded sesquilinear form. By the anti-commutation relations, we have

$$0 \leq \varpi(b(g)b^*(g)) = -\varpi(b^*(g)b(g)) + \|g\|^2,$$

whence $\varpi(b^*(f)b(f)) \leq \|f\|$ is bounded and there exists an operator $\rho \in \mathfrak{B}(\mathfrak{h})$ with $0 \leq \rho \leq 1$ such that

$$\varpi(b^*(f)b(g)) = \langle g, \rho f\rangle_{\mathfrak{h}}. \tag{A.1.8}$$

We call ρ a *single-particle density operator*. The fact that a quasi-free state is fully determined by this density operator corresponds to the physical idea that if the particles do not interact with each other, the state of the many-particle system is a superposition of independent single-particle states. The condition $0 \leq \rho \leq 1$ is sufficient in the sense that any operator ρ on $\mathfrak{h}$ satisfying this relation can be used to define a quasi-free state through (A.1.7) and (A.1.8). Note the following Lemma that states that a quasi-free state remains quasi-free under the evolution $e^{-it\mathrm{d}\Gamma(h)}$ derived from the one particle Hamiltonian h.

Lemma A.1.13. *Let h be a Hamiltonian on the Hilbert space $\mathfrak{h}$ and ϖ a quasi-free state with density operator ρ. Let the time evolution be given by $\mathfrak{t}_t : \mathcal{A}_-(\mathfrak{h}) \to \mathcal{A}_-(\mathfrak{h})$, $\mathfrak{t}_t(A) = e^{it\mathrm{d}\Gamma(h)} A e^{-it\mathrm{d}\Gamma(h)}$ for $t \in \mathbb{R}$. Then $\varpi_t = \varpi \circ \mathfrak{t}_t$ is quasi-free with density operator $\rho(t) = e^{-ith}\rho e^{ith}$ for every $t \in \mathbb{R}$.*

Also, from $\varpi(b^*(f)b(g)) = \langle g, \rho f\rangle$ and Lemma A.1.5, we obtain that for a trace class operator $A = \sum_{j=1}^{\infty} \lambda_j \langle f_j, \cdot\rangle f_j$ on $\mathfrak{h}$ with some orthonormal basis $\{f_j\}_{j\in\mathbb{N}}$ of $\mathfrak{h}$,

$$\varpi(\mathrm{d}\Gamma(A)) = \sum_{j=1}^{\infty} \lambda_j \varpi(b^*(f_j)b(f_j)) = \sum_{j=1}^{\infty} \langle f_j, \lambda_j \rho f_j\rangle = \mathrm{Tr}(A\rho). \tag{A.1.9}$$

A definition similar to (A.1.7) holds for the bosonic case except that the alternating signs of the determinant are all replaced by plus signs. The sesquilinear form $\varpi(a^*(f)a(g))$ is in general unbounded, whence the bosonic density operator does not have to be bounded either. The only condition is that it has to be positive. The equivalent of Lemma A.1.13 holds accordingly.

An example of a gauge-invariant quasi-free sate is the Gibbs grand canonical equilibrium state for a system of particles at inverse temperature β and chemical potential μ described by the single-particle Hamiltonian H. It is given by

$$\varpi_{\beta,\mu}(A) = \mathrm{Tr}_{\mathfrak{F}_\pm(\mathfrak{h})}\big(\zeta_0^{-1} e^{-\beta(\mathrm{d}\Gamma(H)-\mu\mathfrak{N}_\pm)} A\big)$$

with $\zeta_0 = [\mathrm{Tr}\big(e^{-\beta(\mathrm{d}\Gamma(H)-\mu\mathfrak{N}_\pm)}\big)$. Recall Example A.1.8 for bosons, i.e. $\mathfrak{F}_+(\mathbb{C}) = \ell^2(\mathbb{N}_0)$. If $H = \omega\, a^*a$ and $A = \sum_{n\in\mathbb{N}_0} \alpha_n \langle \Upsilon_n, \cdot\rangle \Upsilon_n$ with canonical basis $\{\Upsilon_n\}_{n\in\mathbb{N}_0}$ of $\ell^2(\mathbb{N}_0)$, then $\zeta_0 = (1 - e^{-\beta\omega})^{-1}$ and

$$\varpi_{\beta,\mu}(A) = (1 - e^{-\beta\omega})^{-1} \sum_{n\in\mathbb{N}_0} \alpha_n e^{-\beta n(\omega-\mu)}. \tag{A.1.10}$$

For a general system of independent fermions, one can use the CAR to derive the relation

$$\varpi_{\beta,\mu}(a^*(f)a(g)) = \langle g, f_{FD,\beta}(\lambda - \mu) f\rangle_{\mathfrak{h}}, \tag{A.1.11}$$

where $f_{FD,\beta}(\lambda) = (1 + e^{\beta}\lambda)^{-1}$ is the Fermi-Dirac distribution function.

A.2 Mathematical scattering theory

In this section we give a short introduction into mathematical scattering theory. An in-depth treatment of mathematical scattering theory can be found in the books by Reed and Simon [69], Baumgärtel and Wollenberg [9], and Yafaev [80].

The basic idea of scattering theory is to obtain information on some Hamiltonian H through some simpler Hamiltonian H_0. Usually, H describes a fully interacting quantum system, whence it is called the *coupled* (or *interacting*) Hamiltonian. In contrast, H_0 is called the *decoupled* (or *free*) Hamiltonian. It is similar to H except for all or some of the interaction of the system. To get an idea of the concept, take H_0 as the Hamiltonian of a free electron. Let H describe the same electron subject to a compactly supported potential such that there are no bound states. One expects both electrons to behave similarly for large times $t \to \pm\infty$ since with time they move far away from the interaction region, i.e. the support of the potential. Hence, one expects to find states $g_0, g \in \mathfrak{H}$ such that

$$\lim_{t\to\pm\infty} \|e^{-itH} g - e^{-itH_0} g_0\| = \lim_{t\to\pm\infty} \|g - e^{itH} e^{-itH_0} g_0\| = 0.$$

This is why the strong limit of $e^{itH}e^{-itH_0}$ is of interest and is called the wave operator $W_\pm(H, H_0)$ (see Section A.2.1). The name wave operators derives from the fact that the generalized eigenfunctions of H_0 for free electrons are plain waves that $W_\pm(H, H_0)$ maps to generalized eigenfunctions of H.

Now assume that an electron from far away moves towards the interaction region, passes the region, and then travels far away from the potential. If we know the initial state g_0 of the electron, can we identify the final free state f_0 of the electron that leaves the interaction region? The unitarity of the time-evolution of the system implies that this is the same as asking which state f_0 produces the same asymptotically free state for $t \to +\infty$ as the initial state g_0 for $t \to -\infty$. In other words, we search for an $f_0 \in \mathfrak{H}$ for which

$$W_+(H, H_0) f_0 = W_-(H, H_0) g_0, \qquad \text{i.e.} \qquad \Longrightarrow \qquad f_0 = W_+^*(H, H_0) W_-(H, H_0) g_0.$$

This is the motivation to study the operator $W_+^*(H, H_0)W_-(H, H_0)$, which is called the scattering operator and which contains the information on the transition probabilities that we need for the Landauer-Büttiker formula.

A.2.1 The wave operators and the scattering matrix

After the physical motivation, let us give the rigorous mathematical definition of the wave operators. Note that some vector $v \in \mathfrak{H}$ is the absolute Abelian limit of $v(t) \in \mathfrak{H}$, $t \in \mathbb{R}$, written $v = |\mathrm{A}|\text{-}\lim_{t\to\infty} v(t)$, if and only if $\text{s-}\lim_{t\to\infty} \int_0^\infty \mathrm{d}t\, \epsilon e^{-\epsilon t} \|v(t) - v\|^2$ exists.

Definition A.2.1. *Let H_0, H be two densely defined self-adjoint operators on two Hilbert spaces $\mathfrak{H}_0$ and $\mathfrak{H}$ with domains* $\mathrm{dom}(H_0)$ *and* $\mathrm{dom}(H)$*. The triplet $\{H_0, H, \mathcal{J}\}$ is called a* scattering system*, where $\mathcal{J} : \mathfrak{H}_0 \to \mathfrak{H}$ is the* identification operator*. The* wave operators *$W_\pm(H, H_0, \mathcal{J})$ for the scattering system $\{H_0, H, \mathcal{J}\}$ are defined as the strong limits*

$$W_\pm(H, H_0, \mathcal{J}) = \underset{t\to\pm\infty}{\text{s-lim}}\, e^{itH} \mathcal{J} e^{-itH_0} P_{H_0}^{ac}$$

if the respective limits exist. If the limits are taken as an absolute Abelian limit, which is weaker than the strong limit, we call $W_\pm(H, H_0, \mathcal{J})$ *the* Abel wave operators.

If $\mathfrak{H}_0 = \mathfrak{H}$ *and* $\mathcal{J} = I_{\mathfrak{H}}$*, then we abbreviate* $\{H_0, H\}$ *for the scattering system and* $W_\pm(H, H_0)$ *for the wave operators.*

One can easily show that the strong limit of $e^{itH}\mathcal{J}e^{-itH_0}P^{pp}_{H_0}$ exists if and only if $H = H_0$. Also, the singular continuous spectrum is usually considered to be unphysical. Hence, the choice of $P^{ac}_{H_0}$ in the definition is very natural.

Proposition XI.3.1 of Reed and Simon [69], which we cite below, collects some very interesting and important properties of the wave operators.

Proposition A.2.2. *Let* $\{H_0, H, \mathcal{J}\}$ *be a scattering system such that* $W_\pm(H, H_0, \mathcal{J})$ *exits. The wave operators*

(i) are intertwining, i.e.

$$W \pm (H, H_0, \mathcal{J})\mathrm{dom}(H_0) \subset \mathrm{dom}(H), \qquad W_\pm(H, H_0, \mathcal{J})H_0 = HW_\pm(H, H_0, \mathcal{J}),$$

(ii) are partial isometries with initial space $\mathfrak{H}^{ac}_{H_0}$*,*

(iii) satisfy $\mathrm{ran}(W_\pm(H, H_0, \mathcal{J})) \subset \mathfrak{H}^{ac}_H$*.*

This immediately raises the question if $W_\pm(H, H_0, \mathcal{J})$ are even unitary. In the general case this is not true. It is related to the following definition of completeness.

Definition A.2.3. *Let* $\{H_0, H, \mathcal{J}\}$ *be a scattering system such that the wave operators exist.* $W_\pm(H, H_0, \mathcal{J})$ *are called* complete *if* $\mathrm{ran}(W_\pm(H, H_0, \mathcal{J})) = \mathfrak{H}^{ac}_H$*.*

Completeness states that every scattering state in $\mathfrak{H}^{ac}_H$ is asymptotically free, i.e. the behavior of all non-bound states is essentially described by e^{itH_0} for large times (assuming there is no singular continuous spectrum). It is immediately obvious that if wave operators are complete, then they are surjective isometries, i.e. unitary transformations, as mappings $W_\pm(H, H_0, \mathcal{J}) : \mathfrak{H}^{ac}_{H_0} \to \mathfrak{H}^{ac}_H$. In particular, this implies that the absolutely continuous parts of H_0 and H are unitarily equivalent and this equivalence is provided by the wave operators.

Definition A.2.4. *Let* H *be a densely defined self-adjoint operator on the separable Hilbert space* $\mathfrak{H}$*. A* spectral representation *of* H *is a unitary transformation*

$$\Phi : \mathfrak{H} \to L^2(\mathbb{R}, \mathrm{d}\mathfrak{m}(\lambda), \mathfrak{H}_\lambda)$$

such that $(\Phi Hf)(\lambda) = \lambda(\Phi f)(\lambda)$ *for every* $f \in \mathfrak{H}$ *and* $\mathfrak{m}$*-a.e.* $\lambda \in \mathbb{R}$*.*

Lemma A.2.5. *Let* H *be a densely defined self-adjoint operator on the separable Hilbert space* $\mathfrak{H}$*, and let* Φ *be a spectral representation of* H *on* $L^2(\mathbb{R}, \mathrm{d}\mathfrak{m}(\lambda), \mathfrak{H}_\lambda)$*. For every operator* $Q \in \mathfrak{B}(\mathfrak{H})$ *that commutes with* H*, there is a measurable family of operators* $\{Q(\lambda)\}_{\lambda\in\mathbb{R}}$*, where* $Q(\lambda)$ *acts on* $\mathfrak{H}_\lambda$*, such that* $(\Phi Qf)(\lambda) = Q(\lambda)(\Phi f)(\lambda)$ *for every* $f \in \mathfrak{H}$ *and* $\mathfrak{m}$*-a.e.* $\lambda \in \mathbb{R}$*.*

Let $\Phi_{H_0} : \mathfrak{H} \to L^2(\mathbb{R}, \mathrm{d}\lambda, \mathfrak{H}_\lambda)$ be a spectral representation of H_0^{ac}, the absolutely continuous part of H_0. Using the wave operators, we can define the scattering operator, the transition operator and the corresponding matrices.

Definition A.2.6. *Let $\{H, H_0, \mathcal{J}\}$ be a scattering system such that the wave operators $W_\pm(H, H_0, \mathcal{J})$ exist. The* scattering operator *is defined by*

$$S = W_+^*(H, H_0, \mathcal{J}) W_-(H, H_0, \mathcal{J}).$$

The transition operator *T is given by $S = 1 - 2\pi i\, T$. Since $[S, H_0] = 0$, we have a measurable family $\{S(\lambda)\}_{\lambda \in \mathbb{R}}$ such that*

$$(\Phi_{H_0} S f)(\lambda) = S(\lambda) \widehat{f}(\lambda), \qquad \lambda \in \mathbb{R}, \qquad f \in \mathfrak{H}, \qquad \widehat{f} = \Phi_{H_0} f.$$

We call $S(\lambda)$ the scattering matrix *of $\{H_0, H, \mathcal{J}\}$ with respect to Φ_{H_0}. In the same manner we can define the* transition matrix *$T(\lambda)$.*

We already motivated this definition above. The scattering operator maps a state before the interaction takes place, e.g. an electron far away from the interaction region, to the state that results after the interaction has taken place, e.g. the electron has crossed the interaction region and moved far away from it. If the wave operators are complete, the scattering operator is a unitary operator on $\mathfrak{H}_{H_0}^{ac}$. As a consequence the scattering matrix $S(\lambda)$ is also unitary and we have the following lemma, the so called *optical theorem*.

Lemma A.2.7. *Let $\{H_0, H, \mathcal{J}\}$ be a scattering system such that the scattering matrix is unitary. Then the transition matrix $T(\lambda)$ satisfies*

$$\big(T^*(\lambda) - T(\lambda)\big) = 2\pi i\, T^*(\lambda) T(\lambda)$$

for any $\lambda \in \mathbb{R}$.

Proof. Using $S^*(\lambda) S(\lambda) = I_{\mathfrak{H}(\lambda)}$, we obtain

$$\begin{aligned} T^*(\lambda) T(\lambda) &= -(2\pi i)^{-2} (I_{\mathfrak{H}(\lambda)} - S^*(\lambda))(I_{\mathfrak{H}(\lambda)} - S(\lambda)) \\ &= -(2\pi i)^{-2} (I_{\mathfrak{H}(\lambda)} - S^*(\lambda)) - (2\pi i)^{-2} (I_{\mathfrak{H}}(\lambda) - S(\lambda)) \\ &= 2\pi i \big(T^*(\lambda) - T(\lambda)\big). \end{aligned}$$

□

Note that the intertwining property of the wave operator allows us to define a *wave matrix* $W_\pm(\lambda)$. If Φ_H is a spectral representation of H, we have

$$(\Phi_H W_\pm(H, H_0, \mathcal{J}) \Phi_{H_0}^* \widehat{f})(\lambda) = W_\pm(\lambda) \check{f}, \qquad \lambda \in \mathbb{R}, \qquad f \in \mathfrak{H}, \qquad \check{f} = \Phi_H f.$$

A.2.2 Existence and completeness of wave operators

The central questions when dealing with wave operators are those of existence and completeness. The following fundamental result has first been proven independently by Kato [54] and Rosenblum [71].

Theorem A.2.8. *Let $\{H_0, H, \mathcal{J}\}$ be a scattering system with $\mathcal{J}\mathrm{dom}(H_0) \subset \mathrm{dom}(H)$ and $V = H\mathcal{J} - \mathcal{J}H_0 \in \mathfrak{L}_1(\mathfrak{H})$. Then the wave operators $W_\pm(H, H_0, \mathcal{J})$ exist and are complete.*

Later on, the result has been extended to the case where only the resolvent difference is trace class by Kuroda [59, 60] and Birman [13].

Theorem A.2.9. *Let $\{H_0, H, \mathcal{J}\}$ be a scattering system such that*

$$(H - i)^{-1}\mathcal{J} - \mathcal{J}(H_0 - i)^{-1} \in \mathfrak{L}_1(\mathfrak{H}).$$

Then the wave operators $W_\pm(H, H_0, \mathcal{J})$ exist and are complete.

This result covers a lot of physically interesting situations. For example, the case of the Laplacian perturbed by a compactly supported potential falls into this setting. In higher space dimensions the following generalization of Theorem A.2.9 is often useful (see e.g. [80, Thm. 6.5.1]).

Theorem A.2.10. *Let $\{H_0, H, \mathcal{J}\}$ be a scattering system such that*

$$(H - z)^{-N}\mathcal{J} - \mathcal{J}(H_0 - z)^{-N} \in \mathfrak{L}_1(\mathfrak{H})$$

for some $z \in \mathbb{C} \setminus (\sigma(H) \cup \sigma(H_0))$ and $N \in \mathbb{N}$. Then the wave operators $W_\pm(H, H_0, \mathcal{J})$ exist and are complete.

The wave operators are transitive in a certain sense. This is the content of the following proposition, which is also called the *chain rule* for wave operators (see [69, Prop. XI.3.2]).

Proposition A.2.11. *Let $\{H_0, H_1, \mathcal{J}_1\}$ and $\{H_1, H, \mathcal{J}_2\}$ be two scattering systems such that $W_\pm(H_1, H_0, \mathcal{J}_1)$ and $W_\pm(H, H_1, \mathcal{J}_2)$ exist. Then $W_\pm(H, H_0, \mathcal{J}_2\mathcal{J}_1)$ exists and*

$$W_\pm(H, H_0, \mathcal{J}_2\mathcal{J}_1) = W_\pm(H, H_1, \mathcal{J}_2)W_\pm(H_1, H_0, \mathcal{J}_1).$$

An interesting and important result is the invariance principle, which states that under certain conditions the wave operators for $\{H_0, H, \mathcal{J}\}$ and $\{\varphi(H_0), \varphi(H), \mathcal{J}\}$ are the same. It is due to Wollenberg [79].

Theorem A.2.12. *Let $\varphi : \sigma(H_0) \cap \sigma(H) \to \mathbb{R}$ be piecewise continuously differentiable such that it is a.e. finite with respect to E_{H_0} and E_H, with $\varphi' > 0$ being locally of bounded variation. Let further $\{H_0, H, \mathcal{J}\}$ be a scattering system such that the wave operators $W_\pm(H, H_0, \mathcal{J})$ and $W_\pm(\varphi(H), \varphi(H_0), \mathcal{J})$ exist. Then*

$$W_\pm(\varphi(H), \varphi(H_0), \mathcal{J}) = W_\pm(H, H_0, \mathcal{J}).$$

An important example is the case of operators H_0 and H that are bounded from below. In this case $\varphi(x) = -(x + \theta)^{-N}$ for $\theta > 0$ sufficiently large satisfies the requirements of Theorem A.2.12. Now we assume that $(H + \theta)^{-N} - (H_0 + \theta)^{-N} \in \mathfrak{L}_1(\mathfrak{H})$. Then $W_\pm(H, H_0, \mathcal{J})$ and $W_\pm(\varphi(H), \varphi(H_0), \mathcal{J})$ exist and are complete by Theorem A.2.10, whence

$$W_\pm((H + \theta)^{-1}, (H_0 + \theta)^{-1}, \mathcal{J}) = W_\pm(H, H_0, \mathcal{J}).$$

This can be used to prove results for a scattering system $\{K_0, K, \mathcal{J}\}$ with $K - K_0 \in \mathfrak{L}_1(\mathfrak{H})$ that are then also valid for $\{H_0, H\}$ with $(H+\theta)^{-N}\mathcal{J} - \mathcal{J}(H_0+\theta)^{-N} \in \mathfrak{L}_1(\mathfrak{H})$. We use this concept in our proofs for the Landauer-Büttiker formulae in Chapters 3 and 5. If we can not guarantee the existence of $W_\pm(\varphi(H), \varphi(H_0))$ a-priori, Theorem A.2.12 holds only for the Abel wave operators.

Theorem A.2.13. *Let φ be as in Theorem A.2.12. Furthermore, let $\{H_0, H, \mathcal{J}\}$ be a scattering system such that $W_\pm(H, H_0, \mathcal{J})$ exists as an absolute Abelian limit. Then $W_\pm(\varphi(H), \varphi(H_0), \mathcal{J})$ also exists as an absolute Abelian limit and*

$$W_\pm(\varphi(H), \varphi(H_0), \mathcal{J}) = W_\pm(H, H_0, \mathcal{J}).$$

A.2.3 Stationary scattering theory and operator spectral integrals

The wave operators as they are defined in Definition A.2.1 are usually called the *time-dependent* wave operators since e^{itH} is the solution operator for the Schroedinger equation, t being the time. It is not the only possibility to define the wave operators $W_\pm(H, H_0)$. A second approach is the so called *stationary* scattering theory. The idea is to express the wave operators in terms of stationary objects like the resolvent and the spectral measure instead of the unitary group. This is motivated by the fact that in applications it is usually easier to obtain information on $(H-i)^{-1}$ than on e^{itH}. The presentation of the stationary theory in this section is based on the book by Baumgärtel and Wollenberg [9], especially Chapters III.9 and III.13. The starting point is the definition of the stationary pre-wave operators

$$W_\pm(\epsilon) = \int_0^\infty \mathrm{d}t\, \epsilon\, e^{-\epsilon t} e^{itH} \mathcal{J} e^{-itH_0}, \qquad \epsilon > 0. \tag{A.2.12}$$

We do not concern ourselves with the general theory of the existence of the limit $\lim_{\epsilon\to+0} W_\pm(\epsilon)$. We only mention that if one has no prior information on the existence of the wave operator, one usually considers the case of weak limits since the case of strong limits is considerably harder to handle. For us the following fact that can be found in [9, Prop. III.9.6] is sufficient.

Lemma A.2.14. *If the wave operators $W_\pm(H, H_0)$ exist, then*

$$W_\pm(H, H_0, \mathcal{J}) = \operatorname*{s-lim}_{\epsilon\to+0} W_\pm(\epsilon).$$

The formula (A.2.12) replaces the limit $t \to \pm\infty$ in time with a stationary limit. However, it still contains the unitary group, whence it is not particularly useful to calculate the scattering matrix. The next lemma, taken from [9, Prop. III.13.1], shows that a fully stationary formulation is indeed possible.

Lemma A.2.15. *We have*

$$\langle g, W_\pm(\epsilon) f\rangle = \pm\frac{\epsilon}{\pi}\int_{-\infty}^{\infty} \mathrm{d}\lambda \langle g, (H - \lambda \pm i\epsilon)^{-1}\mathcal{J}(H_0 - \lambda \mp i\epsilon)^{-1} f\rangle$$

for $f, g \in \mathfrak{H}$.

Operator spectral integrals

If one works with strong limits, the weak formulation of Lemma A.2.15 is not the best choice. Using the spectral measure, we can give a more suitable representation. To this end, we have to introduce operator spectral integrals as they can be found in [9, Ch. 5].

Let E_H be the spectral measure of the self-adjoint operator H on $\mathfrak{H}$. For $r > 0$ let $\mathcal{J}_\epsilon^r$ be a partition of $[-r, r)$ into intervals $[r_j, r_{j+1})$ with $|\mathcal{J}_\epsilon^r| = \max_{\Xi\in\mathcal{J}_\epsilon^r}(r_{j+1} - r_j) = \epsilon$. Let $A : \mathbb{R} \to \mathfrak{L}(\mathfrak{H})$ be an operator-valued function and let $\lambda_\Xi \in \Xi$ for $\Xi \in \mathcal{J}_\epsilon^r$. The *operator spectral integral* of A is defined by

$$\int_{\mathbb{R}} A(\lambda)\mathrm{d}E_H(\lambda) = \operatorname*{s-lim}_{r\to\infty}\Big(\operatorname*{n-lim}_{\epsilon\to+0}\sum_{\Xi\in\mathcal{J}_\epsilon^r} A(\lambda_\Xi)E(\Xi)\Big)$$

if the norm-limit $\operatorname{n-lim}_{\epsilon\to+0}$ exists independently of the partitions $\mathcal{J}_\epsilon^r$. Similarly, we can define the operator spectral integral

$$\int_{\mathbb{R}} \mathrm{d}E_H(\lambda)A(\lambda) = \operatorname*{s-lim}_{r\to\infty}\Big(\operatorname*{n-lim}_{\epsilon\to+0}\sum_{\Xi\in\mathcal{J}_\epsilon^r} E(\Xi)A(\lambda_\Xi)\Big).$$

Note that if A is a scalar function, the operator spectral integrals coincide and are equal to the usual spectral integral. Also, for $B \in \mathfrak{L}(\mathfrak{H})$ we have

$$B\int_{\mathbb{R}} A(\lambda)\mathrm{d}E_H(\lambda) = \int_{\mathbb{R}} BA(\lambda)\mathrm{d}E_H(\lambda), \quad \Big(\int_{\mathbb{R}} \mathrm{d}E_H(\lambda)A(\lambda)\Big)B = \int_{\mathbb{R}} \mathrm{d}E_H(\lambda)\big(A(\lambda)B\big).$$

Another useful relation between the usual spectral integral and the operator spectral integral is provided by [9, Prop. I.5.2]. We cite it as a lemma for convenience.

Lemma A.2.16. *If $\int_{\mathbb{R}} A(\lambda)\mathrm{d}E_H(\lambda)$ exists and $a : \mathbb{R} \to \mathbb{R}$ is continuous, then*

$$\int_{\mathbb{R}} a(\lambda)A(\lambda)\mathrm{d}E_H(\lambda) = \int_{\mathbb{R}} A(\lambda)\mathrm{d}E_H(\lambda)\int_{\mathbb{R}} a(\lambda)\mathrm{d}E_H(\lambda),$$

where the left-hand side exists. Similarly, if $\int_{\mathbb{R}} \mathrm{d}E_H(\lambda)A(\lambda)$ exists, then

$$\int_{\mathbb{R}} \mathrm{d}E_H(\lambda)a(\lambda)A(\lambda) = \int_{\mathbb{R}} a(\lambda)\mathrm{d}E_H(\lambda)\int_{\mathbb{R}} \mathrm{d}E_H(\lambda)A(\lambda).$$

The following technical lemma is usefull in Chapter 5.

Lemma A.2.17. *Let $E : \mathcal{B}(\mathbb{R}) \to \mathfrak{L}(\mathfrak{H})$ be a spectral measure. Let $Z : \mathbb{R} \to \mathfrak{L}_1(\mathfrak{H})$ such that $Z'(\lambda)$ exists in the trace norm for a.e. $\lambda \in \mathbb{R}$ and $\|Z'\|_1$ is integrable. Then*

$$\int_{\mathbb{R}} Z(\lambda)\mathrm{d}E(\lambda) \in \mathfrak{L}_1(\mathfrak{H}).$$

Proof. The proof is identical to that of [9, Lemma I.5.4] with the operator norm replaced by the trace norm. □

We can use the operator spectral integrals to give a representation of the wave operators as strong limits of fully stationary terms. This is provided by [9, Prop. III.13.1+2].

Lemma A.2.18. *Let $\{H_0, H, \mathcal{J}\}$ be a scattering system. The stationary pre-wave operators $W_\pm(\epsilon)$, $\epsilon > 0$, from* (A.2.12) *satisfy*

$$W_\pm(\epsilon) = \mp \int_{\mathbb{R}} \mathrm{d}E_H(\lambda)\, i\epsilon \mathcal{J}(H_0 - \lambda \mp i\epsilon)^{-1} P^{ac}_{H_0} = \pm \int_{\mathbb{R}} i\epsilon (H - \lambda \pm i\epsilon)^{-1} \mathcal{J} \mathrm{d}E^{ac}_{H_0}(\lambda).$$

If $\mathcal{J} = I_{\mathfrak{H}}$ and $\mathrm{dom}(H_0) \subset \mathrm{dom}(H)$, then $V = H - H_0$ on $\mathrm{dom}(H_0)$ and

$$W_\pm(\epsilon) = \int_{\mathbb{R}} \mathrm{d}E_H(\lambda)(1 + V(H_0 - \lambda \mp i\epsilon)^{-1}) P^{ac}_{H_0} = \int_{\mathbb{R}} (1 - (H - \lambda \pm i\epsilon)^{-1} V) \mathrm{d}E^{ac}_{H_0}(\lambda). \tag{A.2.13}$$

We close this appendix with a series of technical lemmas that we use in the course of this thesis.

Lemma A.2.19 (Cor. V.18.3, Baumgärtel and Wollenberg [9])**.** *Let $\{H_0, H\}$ be a scattering system with spectral measure $E_0(\cdot)$ and $E(\cdot)$ such that $H = H_0 + V$ and the wave operators exist and are complete. Furthermore, let $g : \mathbb{R} \to \mathfrak{H}$ be such that g and the derivative g' are strongly continuous, $\int_{\mathbb{R}} \mathrm{d}E(\lambda) g(\lambda)$ exists, and $\int_{\mathbb{R}} \|g'(\lambda)\| \mathrm{d}\lambda < \infty$. Then*

$$\int_{\mathbb{R}} \mathrm{d}E_0(\lambda)(1 - V(H - \lambda + i\epsilon)^{-1}) g(\lambda)$$

exists and

$$\begin{aligned} \operatorname*{s-lim}_{\epsilon \to +0} \Bigg(\int_{\mathbb{R}} \mathrm{d}E^{ac}_0(\lambda)(1 - V(H - \lambda + i\epsilon)^{-1}) g(\lambda) \\ - \int_{\mathbb{R}} \mathrm{d}E^{ac}_0(\lambda)(1 - V(H - \lambda + i\epsilon)^{-1}) \int_{\mathbb{R}} \mathrm{d}E(\mu) g(\mu) \Bigg) = 0. \end{aligned}$$

Lemma A.2.20 (Prop. I.1.1+3, Baumgärtel and Wollenberg [9])**.** *Let $\mathfrak{H}$ be a Hilbert space, and let $\varphi \in L^1(\mathbb{R}, \mathfrak{H})$. Then*

$$\operatorname*{s-lim}_{\epsilon \to +0} \int_{\mathbb{R}} \mathrm{d}\eta\, (\eta - \lambda \pm i\epsilon)^{-1} \varphi(\eta) = - \operatorname*{s-lim}_{\epsilon \to +0} \int_{|\eta - \lambda| \geq \epsilon} \mathrm{d}\eta\, (\lambda - \eta)^{-1} \varphi(\eta) \mp i\pi\varphi(\lambda).$$

In particular, we may choose $\mathfrak{H} = \mathfrak{L}_2(\mathfrak{K})$. Also, $\lim_{\epsilon \to +0} \int_{\mathbb{R}} \mathrm{d}\eta\, \frac{\epsilon}{(\eta - \lambda)^2 + \epsilon^2} \varphi(\eta) = \pi\varphi(\lambda)$.

Lemma A.2.21 (Prop. I.3.12-14, Baumgärtel and Wollenberg [9])**.** *Let $C_1, C_2 \in \mathfrak{L}_2(\mathfrak{H})$. Let $E(\cdot)$ be the spectral measure of some self-adjoint $H \in \mathfrak{L}(\mathfrak{H})$. Then $C_1 E(\cdot) C_2$ is an $\mathfrak{L}_1(\mathfrak{H})$-valued measure and it is differentiable in the trace norm. We have*

$$C_1 E(\Xi) C_2 = \int_\Xi \mathrm{d}\mathfrak{m}(\lambda) Y(\lambda)$$

for $Y(\lambda) = \frac{\mathrm{d}}{\mathrm{d}\lambda} C_1 E(\lambda) C_2$ and some nonnegative Borel measure $\mathfrak{m}(\cdot)$. Furthermore,

$$C_1 (H - \lambda \pm i0)^{-1} C_2 = \lim_{\epsilon \to +0} C_1 (H - \lambda \pm i\epsilon)^{-1} C_2$$

exists in the Hilbert-Schmidt norm.

Lemma A.2.22 (Egorov [38]). *Let $(\mathcal{O}, \Sigma, \mathfrak{m})$ be a measure space and let $\{f_n\}_{n\in\mathbb{N}}$ be a sequence of measurable functions on $\mathcal{O}$ converging for $\mathfrak{m}$-a.e. $x \in \mathcal{O}$. Then for every $\epsilon > 0$ one can find a set Ξ with $\mathfrak{m}(\Xi) < \epsilon$ such that $\{f_n\}_{n\in\mathbb{N}}$ converges uniformly on $\mathcal{O} \setminus \Xi$.*

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List of Figures

Selbständigkeitserklärung

Ich erkläre, dass ich die vorliegende Arbeit selbständig und nur unter Verwendung der angegebenen Literatur und Hilfsmittel angefertigt habe.

Berlin, den 26.09.2012 Lukas Wilhelm